SIMULATION OF MULTICOMPONENT DISTILLATION COLUMN

THESIS

Submitted in Partial Fulfillment of the Requirements

for the Award of the Degree of

MASTER OF TECHNOLOGY

(REFINING & PETROCHEMICAL ENGINEERING)

Submitted by

V. AMRNATH REDDY

College of Engineering

University of Petroleum & Energy Studies

Dehradun

May, 2010

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DECLARATION

I hereby declare that the work which is being presented in the thesis entitled "SIMULATION OF MULTICOMPONENT DISTILLATION COLUMN" by "V. AMARNATH REDDY" in partial fulfillment of requirements for the award of degree of M. Tech. (Refining & Petrochemical Engineering) submitted in the Department of Chemical Engineering at UNIVERSITY OF PETROLEUM & ENERGY STUDIES, DEHRADUN is an authentic record of my own work carried out during a period from 1ST NOV, 2010 to 31ST APR, 2010 under the supervision of Prof. K.V. Rao. The matter presented in this thesis has not been submitted by me in any other University / Institute for the award of M. Tech Degree. *Due to the confidentiality of data, the original name, location and identity of the data has been changed.*

Signature of the Student

This is to certify that the above statement made by the candidate is correct to the best of My /our knowledge

Signature of the SUPERVISOR

CERTIFICATE

This is to certify that the work contained in this thesis titled "SIMULATION OF MULTICOMPONENT DISTILLATION COLUMN" has been carried out by Mr. V. AMARNATH REDDY, under my supervision and has not been submitted elsewhere for a degree.

KVIC

Signature of the Supervisor

Date: 11-5-2010

ABSTRACT

In this project, simulation of multicomponent distillation column based on Thiele – Geddes (TG) method has been employed. In fact, TG method is a simulation method and repeated simulations provide a good design. The above method is first algebraic technique for solving steady state multicomponent distillation problems.

The original Thiele – Geddes method is direct iterative method. Therefore an important development was incorporation of matrix methods and convergence techniques. In this work, two types of procedures for accelerating the rate of convergence, classical N-R and 'θ' methods have been used. The 'θ' method was successfully applied with the three variations of TG method to show its advantage. Thomas algorithm is used for solving for tri-diagonal matrix of material balance equations in one of the variations.

The computer programs have been developed by using C++ language. Nine industrial separations, depropanizer-I, parafins (C_9-C_{14}; LAB quality), depropanizer-II, ethane splitter, separation of xylenes, ethyl benzene – styrene, toluene - ethylbenzene, benzene – biphenyl and phenol - crèsols have been used to test the simulation programs developed in this work. The results have been compared with those obtained from HYSYS.

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NOTATION

A_{ji}	absorption factor
A_i	a square matrix for each component i
B	bottom product rate, kg moles/hr
D	distillate/ Top product rate, kg moles/hr
F	feed rate, kgmoles/hr
f_i	a feed vector in the component material balances
f(θ)	function in θ
f'(θ)	derivative of f(θ)
l_{ji}	molar flow rate at which component i in the liquid phase leaves the j th Plate
K	equilibrium constant
L	liquid phase flow rate, kg moles/hr
M	as defined in eq.52
N	total number of plates
NC	number of components
NR	number of stages in rectifying section
NS	number of stages in stripping section
P_i	vapor pressure of component i, mmHg
P	total pressure, mmHg
R	reflux ratio
T	equilibrium temperature, °C
V	vapour phase flow rate, kg moles/hr
v_{ji}	molar flow rate at which component flow rates in the vapour leaves plate j
v_i	column vector of components flow rates in the vapour phase;
x	liquid phase mole fraction
y	vapor phase mole fraction

SUBSCRIPTS

b	base component
B	bottom product
cal	calculated
cor	corrected
D	distillate or top product
F	feed
f	feed plate
itr	iteration number
R	rectifying section
S	stripping section
i	component number
j	stage number; for the accumulator j=0; for the top plate j=1, for the feed plate j=f, for the bottom plate j = N, and for the reboiler , j = N +1;

GREEK SYMBOLS

α	relative volatility
ρ_{ji}	defined as $(1+A_{ji})$
θ	a multiplier in θ convergence method

1. INTRODUCTION

1.1 MULTICOMPONENT DISTILLATION

Multicomponent distillation is widely used in petroleum refining and petrochemical industries. In petroleum refining, it is known as complex distillation as the separation of liquid mixtures is not based on specific components but on the pseudo components (which are cuts or fractions of the mixture having different average boiling points). In the design of a multicomponent distillation (a single feed stream+ top and bottom product streams), it is generally possible to specify the separation between any two components in the mixture. In binary distillation design, two specifications can determine the compositions of the top and bottom products streams, whereas the specification of two components will not sufficient to fix the entire composition of the product streams in the multicomponent distillation. If the distribution of two components called key components between the top and bottom products are specified, the distributions of other components in both the product streams will be determined by the design conditions chosen to accomplish the specified separation of the key components. More volatile key component in the mixture is termed as light key and the less volatile key component as heavy key.

Sometimes, even the mole fractions of both light and heavy components in the products are specified, the specification might be acceptable, but the specified values could not be achieved with any number of theoretical plates or any reflux rates. As such the simultaneous solution of several equations describing the material and energy balances and the vapour liquid equilibrium relationships in multicomponent distillation column is much more different than it is for a binary distillation column.

Before 1950's, column calculations were performed by hand although rigorous calculation procedures were available, they where difficult to apply for all but very small columns. Short cut methods where therefore the primary design tool. Rigorous procedures were only used for small columns or for final design checks. Inaccuracies and uncertainties in the shortcut procedures were usually accommodated by overdesign.

The introduction of computers has entirely reversed the design procedure. Rigorous calculations, once taking several days, sometimes weeks, for even a simple column, can now be performed quickly and efficiently using a computer. No longer is there a need to tolerate

inaccuracies and uncertainties inherent in the shortcut procedures. In modern distillation practice, rigorous methods are the primary design tool.

The use of computers also led to a rapid development of better rigorous procedures. The rigorous methods developed in the 1930s were replaced by more efficient methods. Further, developments took place to permit application of rigorous methods to many complex fractionators, some of which could not be adequately modelled by shortcut methods.

With the superior accuracy and capabilities of modern rigorous methods, a column should not be designed without them. A shortcut calculation is inferior in accuracy, and in some cases may give misleading results. In most modern column design work, the role of shortcut calculations is restricted to eliminating the least desirable design options, providing the designer with an initial estimate for the rigorous step and for troubleshooting the final design. The rigorous methods are used as the primary design and optimization tool.

1.2 DESIGN AND SIMULATION METHODS

In the design method, the goal is to determine the number of plates needed and the location of the feed plate along with specification of the following variables. First separation variable e.g., the recovery of the light key component in the top (distillate) product and the second separation variable e.g., the recovery of the heavy key component in the bottom product. The criterion of feed plate is used to minimize the total number of plates.

In the simulation method, the goal is to determine the compositions of the top and bottom products and the following is generally specified:

- The number of plates above the feed plate.
- The number of plates below the feed plate
- One external flow, such as the flow rate of the top product.
- One internal flow, such as the reflux flow from the condenser (or the reflux ratio).

Two methods are employed in the design of multicomponent component distillation columns. They are i) the Lewis-Matheson method and the Thiele-Geddes method. The Lewis-Matheson method is a design method and the Thiele-Geddes method is a rating or simulation method. Repeated simulations will result in fixing design variables for the desired separation of the key components.

Thiele-Geddes method involves guessing a temperature profile in the column, then performing a procedure much like the stage-to-stage method described above, except that ratios of flow rates (such as vi /di or vi/bi) are determined initially and then a matching procedure at the feed plates permits the determination of compositions everywhere in the column. The calculated compositions facilitate to estimate an improved temperature profile and the procedure is repeated to achieve an improved solution. Convergence is achieved when the temperature profile does not change from iteration to iteration.

1.3 DEVELOPMENT OF THIELE-GEDDES (TG) METHOD

Multicomponent steady state distillation calculations are generally extremely laborious when made without the use of computer. For this reason, work in the past was directed toward correlations and empirical short-cut techniques. Perhaps the best known of these are the charts prepared by Brown & Martin [1] and Gilliland [2].

When simplifying assumptions i.e, constant relative volatilities and fluid rates are applicable, analytical solution of the problem with one feed and two product streams is possible. This was anticipated by Harbert [3], and developed independently by Underwood [4] and Murdock [5].

The computer application procedures for the method have been developed based on the articles of several researchers. Amundson & Pontinen [21], Lyster et al [22], Holland [23,16], Friday & Smith [24], Wang & Henke [25], Napthali and Sandholm [26], Tomich [27], Billingsley [28], Boston and Sullivan [29]. A series of programs for the solution of problems in distillation, extraction, stripping and absorption, which use an iterative procedure similar to the Thiele-Geddes method are given by Hanson et al. [6]. Earlier TG methods are based on solving nest of material balance equations and the latter methods are based on matrix methods, especially tridiogonal matrix methods. The various solving methods are reviewed by Henley and Seader [7] and Kister [8] and discussed in several handbooks [9, 10, 11, 12, 13 & 14] and explained with stage by stage calculation in Perry's hand book [13]. With the Thomas algorithm [15] to solve the material balance equations, efficient convergence procedure, the so-called "theta method" coupled with Kb method for revising the temperature profile and constant composition method to update the phase flow rates as suggested by Holland [16], the modern TG method is found to be powerful in dealing with most of the simulations in multicomponent distillation design.

Aronofsky [30], Bonner [31, 19], Hanson[6], McIntire and Shelton [32, 33], among others, applied the Lewis-Matheson Method on computers for the calculation of conventional fractionators. Bard and Greenstadt [34, 35] employed the Newton-Raphson method for the simultaneous solution of the system of equations used in the Lewis-Matheson method. These authors claimed that their method worked for both conventional and complex columns. There is generally no assurance that the Newton-Raphson method would converge. Wang and Henke [17] employed the tridiagonal matrix algorithm to overcome the convergence problems.

With any computer method of solution, a difficulty which arises is the method employed in mixing the necessarily initial assumptions. As time of computation is usually of paramount importance, judicious initial assumptions can be quite advantageous. The time of computation may be reduced by a large factor by assumptions and/or temperature. Bonner [18, 19] attempted to reduce the time of computations using the Gilliland [20] short-cut technique.

1.4 PRESENT STUDY

In the present study, computer Programs have been developed for 4 variations of the TG method in 'C ++' to simulate the multicomponent distillation columns with an assumption of constant molal flow in the two sections, rectifying and stripping sections of a conventional distillation column. The standard examples have been chosen to test the programs and compare the results of present work with the results of Hysys. The variations of TG method along with procedures adopted, the code of the programs, the details of the examples, the results are presented in the subsequent chapters. In the final Chapter, the results are analyzed and discussed.

2. VARIATIONS OF THIELE-GEDDES METHOD

2.1 THIELE- GEDDES METHOD

This is one of the first rigorous methods for distillation and is the basis of most modern rigorous methods. A key point of the Thiele- Geddes method is the use of the absorption and stripping factors. These will appear in the computer methods. It is known as the rating method because it requires the specification of all feed conditions, feed stage locations, reflux rate, total products rates, and number of stages. Product compositions and exchangers duties are calculated.

The original form of the Thiele-Geddes method uses the stripping and absorption factors to calculate liquid and vapour compositions. The compositions for the rectifying sections are calculated stags to stage by successive substitution, beginning with the distillate product, until the feed stage is reached.

Compositions for the stripping section are found by the same procedure, but beginning with the reboiler and calculating up to the feed. With these compositions, the temperatures are updated, usually by a trial and error bubble point technique. With the new temperatures, the total flow rates are calculated from the energy balance. A test is then made of overall total and component balances. If the column is the out of balance, the top and bottom compositions are adjusted and the calculation is repeated.

2.2 DEVELOPMENT OF COMPUTER PROGRAMS

In the present endeavor, four variations of TG method have been studied. These variations are summarized in Table-1

In all the four variations the material balance equations consisting of the following group of state variables (independent) are solved. The first three programs are developed on the basis of liquid compositions and the subsequent programs on the basis of component flow rates. All the plates are assumed to ideal.

- Plate temperature T_j 's
- Internal total and vapor liquid rates, V_j's and L_j's are held constant in each section.
- Plate compositions $y_{i,j}$'s and $x_{i,j}$'s or component flow rates , $v_{i,j}$'s and $l_{i,j}$'s

Table - 1: Details of Variations Used in the programs

Variation	1	2	3	4
Constant molal flow	✓	✓	✓	✓
Material balance equations based on component flow rates	×	×	×	✓
Material balance equations based on compositions	✓	✓	✓	×
Theta convergence method	×	✓	✓	✓
Thomas algorithm	×	×	×	✓
Correction of temperature by Kb method	×	×	✓	✓
Correction of temperature by bubble point method	✓	✓	×	×
Equilibrium values, K	✓	✓	✓	×
Absorption factors only	×	×	×	✓

1=TGXBP: Thiele-Geddes Composition Bubble Point; 2= TGXBPTH: Thiele-Geddes Composition Bubble Point Theta method; 3=TGXKBTH: Thiele-Geddes Composition KB method Theta method; 4= TGCKBTTH: Thiele-Geddes Component flow rate KB method Theta method

✓: yes; ×: no

Bubble point method has been used to correct the temperatures in the first, and second programs, while KB method has been employed in third and fourth programs.

The θ method of convergence is common in all the versions except for the first program. In the 4th version, the tri-diagonal matrix of the component flow rates for all the plates is solved using the Thomas- Algorithm. K values calculated from Antoine equations are used in all the four versions studied in this work. As the programs are employed to simulate low pressure multicomponent separation of nearly ideal mixtures, the K-value calculation from the pure component vapor pressures is justified.

The following variables are specified: column pressure, type of condenser (partial or total), number of plates in rectifying section as well as in the stripping section, reflux ratio (L/D), feed rate, feed composition. The phase flow rates are assumed to be constant in each section of the column. The temperature profile of the entire column, which is the independent variable, is assumed initially and is modified by plate-to-plate calculations until a good agreement is reached between the assumed and calculated values. At the end of the iterative calculations, the distillate (top) and bottom (residue) compositions and the temperature profile and composition profiles are obtained when the convergence criteria is achieved.

A step wise procedure for the first program is described below. In the appropriate steps, variations are introduced and the programs are developed in similar manner. The method of

each variation is given Appendix-I. As the programs are simple to understand, the step-wise procedure for the other programs are not presented.

2.3 METHDOLOGY

The schematic diagram of the distillation column is shown in the Figure 1. It consists of a total condenser and N plates. The reboiler is considered as an equilibrium plate, N+1. As the product compositions are unknown, the compositions (both vapour and liquid) of the rectifying section and stripping section are expressed as the ratios of mole fractions i.e., $x_{i,r}/x_{i,D}$, $y_{i,r}/y_{i,D}$ and $x_{i,s}/x_{i,B}$, $y_{i,s}/y_{i,B}$. The exact values of the compositions are established only at the end of the iterative plate to plate calculation procedure.

The calculations are initiated from the top plate in the rectifying section and continued till the feed plate is reached to have the values of the ratio of$x_{i,r}/x_{i,D}$, $y_{i,r}/y_{i,D}$ Then, the computations are performed from the reboiler to the feed plate to obtain the ratio of mole fractions $x_{i,s}/x_{i,B}$ and $y_{i,s}/y_{i,B}$. By matching the ratios of mole fractions of the feed plate calculated from the top and bottom sections, the values of the ratios of the compositions of all the components of the top and bottom products are obtained. Thus,

$$(x_{i,B}/x_{i,D})_{cal} = (x_{i,F}/x_{i,D})\,(x_{i,F}/x_{i,B}) \quad (1)$$

The above composition ratios are used to calculate $x_{i,D}$, $x_{i,B}$ as follows:

$$(x_{i,D})_{cal} = F * x_{i,F}/(D + B * (x_{i,B}/x_{i,D})_{cal}) \quad (2)$$

$$(x_{i,B})_{cal} = (x_{i,B}/x_{i,D})_{cal} * (x_{i,D})_{cal} \quad (3)$$

To improve temperature profile in each iteration, the corrected mole fractions for the liquid and vapour phase mole fractions of all the components on each plate are calculated as follows:

$$x_{i,j} = (x_{i,j}/x_{i,D})_{cal} * (x_{i,D})_{cal}/\Sigma(x_{i,j}/x_{i,D})_{cal} * (x_{i,D})_{cal} \quad (4)$$

$$x_{i,j} = (x_{i,j}/x_{i,B})_{cal} * (x_{i,B})_{cal}/\Sigma(x_{i,j}/x_{i,B})_{cal} * (x_{i,B})_{cal} \quad (5)$$

The concept of bubble point temperature is used to calculate the new temperature profile. When the liquid composition is known, the temperature, at which the sum of vapour compositions calculated as Σ Kx should be equal to 1 on each plate, is the bubble point

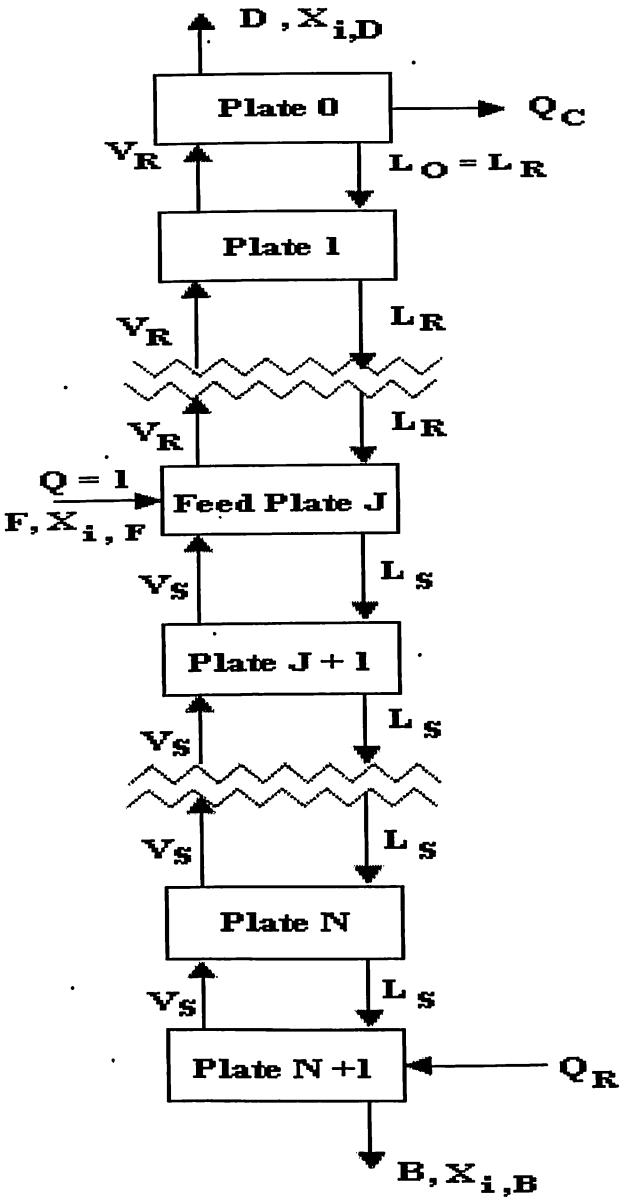

Figure1: Configuration of a conventional distillation column with liquid and vapor streams including product streams for the programs

temperature of the plate. After getting the revised temperature profile, the calculations are repeated till the convergence is achieved. The stepwise procedure is given below.

2.3.1 Stepwise Procedure

1. Specify the following variables
   - i. Number of components in the liquid mixture for separation, NC
   - ii. Feed rate, F: composition of each component, $X_{i,F}$, saturated liquid feed Q=1
   - iii. Product recovery, D/F or B/F;

iv. Number of stages in rectifying section, NR

Number of stages in stripping section, NS

Feed plate location, NF

Total number of plates, NP=NS+NR+2

v. Reflux ratio, R. The reflux is assumed to be saturated liquid.

vi. Liquid and vapor flow rates in the rectifying and stripping section are assumed (RL and RV in rectifying section.

RL=D*R; RV=L+D; SL=RL+Q*F ; SV= RV-(1-Q) *F

vii. Type of condenser :total

viii. Top pressure of the column and allowable pressure drop per plate,

ix. 'K' values as function of T for all the components at the given pressure

2. Assume a linear temperature and pressure profile of the column.

i. Calculate bubble point and dew point temperature for the assumed compositions of the bottom and top product. The temperatures may be taken as the initial bottom temperature (Reboiler temperature or Nth plate temperature) and top temperatures. Alternatively, if the key components are significant (Heavy key in the bottom product and light key component in the top product), the boiling temperatures of these components at the given pressure may be taken as the initial bottom (T_{Bot}) and top temperature (T_{Top}).

ii. Calculate ΔT

$$\Delta T = (T_{Bot} - T_{Top})/(NP - 1) \quad (6)$$

iii. Calculate each plate temperature in the column

$$T_j = T_{j-1} + \Delta T \quad \text{(j=2, NP)} \quad (7)$$

3. Calculate the pressure of each plate for given condenser pressure, top plate pressure and ΔP

$$P_j = P_{j-1} + \Delta P \quad \text{(j=2, NP)} \quad (8)$$

4. Calculate the values of equilibrium constant,$K_{i,j}$ for each component on each plate.(If K_i is function of both temperature and pressure, then correlation for each component may be used)

$$K_{i,j} = exp[A_i - (B_i/T_i + C_i)]/P_i \quad \text{(j=1, NP; i=1, NC)} \quad (9)$$

5. Initialize the ratios of the compositions $y_{i,1}/x_{i,D}$ and $y_{i,NP}/x_{i,B}$

$$y_{i,1}/x_{i,D} = 1 \quad \text{(i=1, NC)} \quad (10)$$

$$y_{i,NP}/x_{i,B} = K_{i,NP} \quad \text{(i=1, NC)} \quad (11)$$

6. Calculate the values of the ratios of the components for each plate in the rectifying section.

$$x_{i,j}/x_{i,D} = (y_{i,j}/x_{i,D})/K_{i,j} \quad \text{(j=1, NR; i=1, NC)} \quad (12)$$

$$y_{i,j+1}/x_{i,D} = [RL * (x_{i,j}/x_{i,D}) + D]/\, RV \quad \text{(j=1, NR; i=1, NC)} \quad (13)$$

7. Calculate the ratios of compositions, $x_{i,j}/x_{i,B}$ and $y_{i,j}/x_{i,B}$ for each component on each plate in the stripping section.

$$x_{i,NP-j}/x_{i,B} = [SV * (y_{i,NP-j+1}/x_{i,B}) + B]/\, SL \quad \text{(j= 1, NS+1; i=1, NC)} \quad (14)$$

$$y_{i,NP-j}/x_{i,B} = K_{i,NP-j} * x_{i,NP-j}/x_{i,B} \quad \text{(j= 1, NS+1; i=1, NC)} \quad (15)$$

8. Calculation of the ratio compositions, $(x_{i,B}/x_{i,D})$

$$x_{i,B}/x_{i,D} = (x_{i,NF}/x_{i,D})\,(x_{i,NF}/x_{i,B}) \quad \text{(i=1, NC)} \quad (16)$$

9. Calculate the top product composition $X_{i,D}$ from the overall component balance of the column and then $X_{i,B}$.

$$x_{i,D} = F * x_{i,F}/(D + B * (x_{i,B}/x_{i,D})) \quad \text{(i=1, NC)} \quad (17)$$

$$x_{i,B} = (x_{i,B}/x_{i,D}) * x_{i,D} \quad \text{(i=1, NC)} \quad (18)$$

10. Normalize the product compositions, $x_{i,D}$ and $x_{i,B}$

$$x_{i,D\,CAL} = x_{i,D}/\,\Sigma\, x_{i,D} \quad \text{(i=1, NC)} \quad (19)$$

$$x_{i,B\,CAL} = x_{i,B}\,/\,\Sigma\, x_{i,B} \quad \text{(i=1, NC)} \quad (20)$$

11. Obtain the liquid compositions of all the components on each plate.

i. Rectifying section

$$x_{i,j} = (x_{i,j}/x_{i,D}) * x_{i,D\,CAL} \quad \text{(j=1, NR; i=1, NC)} \quad (21)$$

ii. Stripping section

$$x_{i,NP-j} = (x_{i,NP-j}/x_{i,B}) * x_{i,B\,CAL} \quad \text{(j=1, NS+1; i=1, NC)} \quad (22)$$

12. Normalization of the liquid compositions on each plate in the column

$$x_{i,j} = x_{i,j}/\Sigma x_{i,j} \quad \text{(j=1, NP; i=1, NC)} \quad (23)$$

13. Correct the temperature profile using bubble method.

i. $K_{i,j} = exp[A_i - (B_i/T_i + C_i)]/P_i$ (j=1,NP ; i=1, NC)

ii. Calculate the $y_{i,j} = K_{i,j} * x_{i,j}$ (j=1,NP; i=1, NC)

iii. Calculate sum of $y_{i,j}$ (j=1,NP; i=1,NC)

iv. F = sumy-1

v. If Absolute value of F is less than an error tolerance of 10^{-4} or 10^{-6}, T[j] is corrected by using Newton's method.

vi. T[j] = T[j] – F/DF. Where DF is derivative of F in Temperature.

vii. Then the calculation is repeated from (i) to (VI) until the condition in (v) is satisfied.

14. Change the iteration number.

iter =iter+1;

Repeat the calculations from the step3. No convergence procedure used except for 20 or more iterations. After convergence, plate compositions and temperature are obtained along with the values of $x_{i,D}$ and $x_{i,B}$.

2.3.2 The 'θ' Method of Convergence

Theta method of convergence is recommended for solving problems involving any type of distillation column; provided that the mixtures do not deviate too widely from ideal solutions. For such columns, the θ method is one of the fastest known methods.

This method has been primarily applied to the Thiele-Geddes equations but a form of the theta method equation has also been applied to the equations of the Lewis-Matheson method. To achieve fast convergence of the problems dealing with the simulation of distillation columns, the 'θ' method combined with K_b method was proposed by Holland [23, 24]. To show the complete understanding of these methods, the equations and Thomas algorithm have been taken from the above mentioned reference of Holland.

The main independent variable of the method is a convergence promoter, theta (or θ). The convergence promoter θ is used to force an overall component and total material balance and to adjust the composition on each stage. In the iterative procedure, the improved sets of liquid mole fractions on each plate in a column required for the calculation of a new temperature profile are obtained using the corrected product compositions (top and bottom).The corrected product rates are used as weight factors in the calculation of mole fractions. The corrected terminal rates are selected such that they are both in overall component material balance and in agreement with the specified value of D, that is

i. The overall component material balance and

$$Fx_{F,i} = (d_i)_{co} + (b_i)_{co} \tag{24}$$

ii. The criterion of the sum of the top product compositions, which is equal to unity.

$$\sum_1^{NC}(d_i)_{co} = D \tag{25}$$

These two conditions must satisfied simultaneously by suitable choice of the multiplier θ, which is defined by

$$(b_i/d_i)_{co} = \theta(b_i/d_i)_{ca} \tag{26}$$

The subscripts co and ca are the corrected and calculated values of a variable, respectively.

Elimination of $(b_i/d_i)_{ca}$ from Eqs (25) and (26) yields the formula for $(d_i)_{co}$.

$$(d_i)_{co} = Fx_i/[1 + \theta(b_i/d_i)_{ca}] \tag{27}$$

Since the specified values of $(d_i)_{co}$ are to have a sum equal to the specified value of D, the desired value of θ is that θ > 0 that makes g(θ) = 0, where

$$g(\theta) = \sum_1^{NC}(d_i)_{co} - D \tag{28}$$

In the determination of θ by Newton's method, the following formula for the first derivate, $g'(\theta)$, is need.

$$g'(\theta) = \sum_1^{NC}(b_i/d_i)_{ca}Fx_i/[1 + \theta(b_i/d_i)_{ca}]^2 \tag{29}$$

After the desired value of θ has been obtained, $(b_i)_{co}$ may be computed by use of Eqa (26). Since Newton's method converges to the positive root of g(θ), provided θ=0 is taken to be the first trail value.

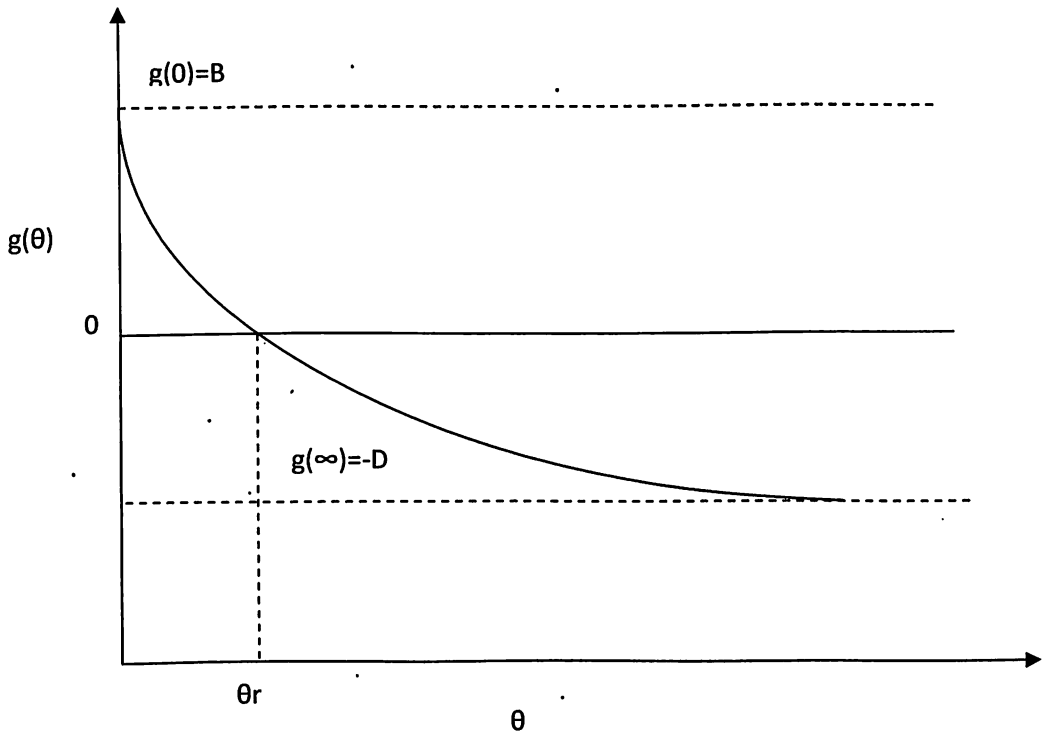

Figure 2: Geometrical Representation of the function g(θ) in the neighbourhood of the positive root θ.

The corrected mole fractions for the liquid and vapour phases are computed as follows

$$x_{j,i} = \left(l_{j,i}/d_i\right)_{ca}(d_i)_{co}/\sum_1^{NC}\left(l_{j,i}/d_i\right)_{ca}(d_i)_{co} \quad (30)$$

$$y_{j,i} = \left(v_{j,i}/d_i\right)_{ca}(d_i)_{co}/\sum_1^{NC}\left(v_{j,i}/d_i\right)_{ca}(d_i)_{co} \quad (31)$$

2.3.3 The K_B method

Robinson and Gilliland pointed out that if the relative values of the $K_i's$ or $P_i's$ are independent of temperature, the trial and error calculations are avoided in the determination of bubble-point and dew-point temperatures. The ratio K_i/K_b is called the relative volatility α_i of component I with respect to component b, that is

$$\alpha_i = K_i/K_b \quad (32)$$

Where K_i and K_b are evaluated at the same temperature and pressure. Component b may or may not be a member of the given mixture under consideration.

When the x_i and pressure Pare given and it is desired to determine the bubble-point temperature, the formula needed may be developed as follows

$$y_i = (K_i/K_b)K_b x_i = \alpha_i K_b x_i \quad (33)$$

Summation of the members of above Eq (33) over all components i, followed by rearrangement yields

$$K_b = 1/\sum_1^{NC} x_i\,\alpha_i \quad (34)$$

Since $\alpha_i's$ are independent of temperature, they may be computed buy use of the values of K_b and K_i evaluated at any arbitrary value of T and at the specified pressure. After K_b has evaluated by use of Eq (34), the desired bubble-point temperature is found from the known relationship between K_b and T.

If the y_i are known instead of the$x_i's$, then the desired formula for the determination of the dew-point temperature is found by rearranging the Eq (34) to the following form

$$K_b x_i = y_i/\alpha_i \quad (35)$$

and then summing over all components to obtain

$$K_b = \sum_{i=1}^{c} y_i/\alpha_i \quad (36)$$

This Eq (36) is used to determine the dew-point temperature in a manner analogous to that described to determine the bubble point temperature.

Many families of compounds are characterized by the fact that their vapor pressures may be approximated by the Clausius-Clapeyron equation, and by the fact that their latent heats of

vaporization are approximately equal. The logarithm of the vapor pressures of the members of such families of compounds falls on parallel lines when plotted against the reciprocal of the absolute temperature. For any two members i and b of such a mixtures, it is readily shown that α_i is independent of temperature.

Although there exists many systems whose $\alpha_i's$ are very nearly constant and Eqs (34) and (36) are applicable for the determination of the Bubble-point and Dew-point temperatures, respectively, the greatest use of these relationships lies in their application in the iterative procedures for solving multicomponent distillation problems.

This method replaces the bubble point method in some of the programs. The new temperature profile for the next iteration is calculated on the basis of the corrected liquid mole fractions and the temperature profile of the previous iteration by using the K_B method. This method is considered as a modified bubble point method. For any plate, Eq (34) may be applied as follows

$$(K_{j,b})_{T_{j,n+1}} = 1/\sum_{i=1}^{c}(\alpha_{j,i})_{T_{j,n}} x_{j,i} \tag{37}$$

Where, $\alpha_{j,i} = K_{j,i}/K_{j,b}$, the relative volatility of component i at the temperature of plate j , and $K_{j,b}$ is the K value of base component (in the calculations , heavy key component is considered as the base component. As the value of $K_{j,b}$ is function of temperature . The new temperature of each plate can be calculated using K equation rewritten for T.

$$T_j = [b_i/(a_i - \log(K_{j,b} * P_j)] - c_i \tag{38}$$

2.3.4 Tridiagonal matrix method

The Tridiagonal Matrix Method, introduced by Wang and Henke [25] is a fast and accurate technique for calculating the component and total flow rates. This method for calculating the component flow rates is used in most of the rigorous methods.

$$\left.\begin{aligned}
&y_{i,j} = x_{i,j} * K_{i,j}\\
&\sum y_{i,j} = 1\\
&\sum x_{i,j} = 1\\
&V_{j+1}y_{j+1,i} = L_j x_{j,i} + D * x_{D,i} \qquad (j=1, 2\ldots f\text{-}1)\\
&V_f y_{f,i} + V_F y_{F,i} = L_{f-1}x_{f-1,i} + D.* x_{D,i}\\
&V_{j+1}y_{j+1,i} = L_j x_{j,i} - B * x_{B,i} \qquad (j=f, f+1\ldots N\text{-}1)\\
&FX_i = D * X_{D,i} + B * X_{B,i}
\end{aligned}\right\} \tag{39}$$

The equations utilized in this procedure differ in form from those presented by Eq.39, they are equivalent independent set. In the case of component material balances, a new set of variables-the component flow rates in the vapor and liquid phases are introduced, namely,

$$v_{ji} = V_j y_{ji} \text{ and } \qquad l_{ji} = L_j x_{ji} \tag{40}$$

Also, the flow rates of component i in the distillate and bottoms are represented by

$$d_i = D\, x_{Di} \text{ and } \qquad b_i = B\, x_{Bi} \tag{41}$$

And the flow rates of component i in the vapor and liquid parts of the feed by

$$v_{Fi} = V_F y_{Fi} \text{ and } \qquad l_{Fi} = L_F x_{Fi} \tag{42}$$

The equilibrium relationship rewrite in terms of the component-flow rates and as follows. Then, expression may be restated in the form

— — (43)

Or and

The absorption factor and the stripping are defined as follows

(44)

An equivalent set of component-material balances is obtained by enclosing each stage (j=1, 2... N, N+1) by a component-material balance

The set of material balance for each component i are as follows

$$\left.\begin{aligned}
&-l_{1i} - d_i + v_{2i} = 0 \\
&l_{1i} - v_{2i} - l_{2i} + v_{3i} = 0 \\
&l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0, \text{ (j=2, 3...., f-2)} \\
&l_{f-2,i} - v_{f-1,i} - l_{f-1,i} + v_{fi} = -v_{Fi} \\
&l_{f-1,i} - v_{fi} - l_{fi} + v_{f+1,i} = -l_{Fi} \\
&l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0, \text{ (j=f+1, f+2...., N-1)} \\
&l_{N-1,i} - v_{N,i} - b_i = 0
\end{aligned}\right\} \tag{45}$$

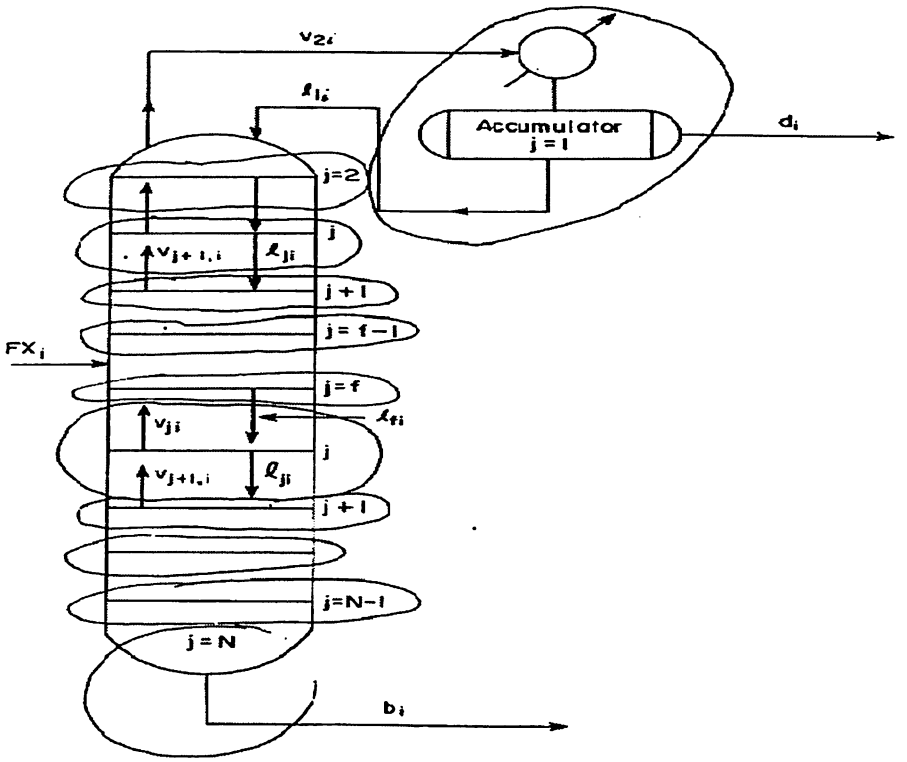

Figure 3: Representation of the component material balance given by Eq (39)

For a partial condenser, $y_{1,i} = x_{D,i}$ and hence $y_{1,i} = x_{1,i} * K_{1,i}$ may be restated as follows

$$Dx_{Di} = (\frac{DK_{1,i}}{L_1})L_1 x_{1,i}$$

$$\text{Or} \qquad l_{1,i} = A_{1,i} d_i \tag{46}$$

Where $A_{1,i} = \frac{L_1}{K_{1,i} D}$ (47)

The expression given by Eq 46 may be used to represent both a partial condenser and a total condenser, provided that $A_{1,i}$ is set equal to L_1/D for a total condenser. Also, the form of $A_{N,i}$ differs slightly from that for A_{ji} because of the double representation of the Reboiler by the subscripts N and B. Thus, the equilibrium relationship $y_{N,i} = x_{N,i} * K_{N,i}$ may be restated in the form

$$V_N y_{N,i} = (\frac{K_{N,i} V_N}{B}) B x_{B,i}$$

$$\text{Or} \qquad b_i = A_{N,i} v_{N,i} \tag{48}$$

Where $A_{N,i} = \frac{B}{K_{N,i} V_N}$ (49)

When the 's and b_i are eliminated from the above MB equations, the following result is obtained

$$\left.\begin{aligned}
&-(A_{1,i}+1)d_i + v_{2,i} = 0\\
&A_{1,i}d_i - (A_{2,i}+1)v_{2,i} + v_{3,i} = 0\\
&A_{j-1,i}v_{j-1,i} - (A_{ji}+1)v_{ji} + v_{j+1,i} = 0,\ (j=3,\ 4\ldots.,\ f\text{-}2)\\
&A_{f-2,i}v_{f-2,i} - (A_{f-1,i}+1)v_{f-1,i} + v_{fi} = -v_{Fi}\\
&A_{f-1,i}v_{f-1,i} - (A_{fi}+1)v_{fi} + v_{f+1,i} = -l_{Fi}\\
&A_{j-1,i}v_{j-1,i} - (A_{ji}+1)v_{ji} + v_{j+1,i} = 0,\ (j=f+1,\ f+2\ldots.,\ N\text{-}1)\\
&A_{N-1,i}v_{N-1,i} - (A_{N,i}+1)v_{N,i} = 0
\end{aligned}\right\} \quad (50)$$

This set of equations may be stated in the matrix form

$$A_i v_i = -f_i \quad (51)$$

Where

$$A_i = \begin{bmatrix}
-\rho_{1i} & 1 & 0 & 0 & \cdots & \cdots & \cdots & 0\\
A_{1i} & -\rho_{2i} & 1 & 0 & \cdots & \cdots & \cdots & 0\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
0 & 0 & A_{f-2,i} & -\rho_{f-1,i} & 1 & 0 & 0 & 0\\
0 & 0 & 0 & A_{f-1,i} & -\rho_{fi} & 1 & 0 & 0\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
0 & \cdots & \cdots & \cdots & 0 & A_{N-2,i} & -\rho_{N-1,i} & 1\\
0 & \cdots & \cdots & \cdots & 0 & 0 & A_{N-1,i} & -\rho_{Ni}
\end{bmatrix}$$

$$v_i = [d_i, v_{2,i} v_{3,i} \ldots v_{f-1,i} v_{f,i} \ldots v_{N-1,i} v_{N,i}]^T$$

$$f_i = [00\ldots 0 v_{Fi} l_{Fi} 0\ldots 00]^T$$

$$\rho_{ji} = (1 + A_{ji})$$

The calculation procedure is initiated by the assumption of a set of temperatures and a set of vapour rates from which the corresponding set of liquids rates is found by use of total material balance presented below.

This particular choice of independent variables was first proposed by Thiele-Geddes. On the basis of the assumed temperatures and flow rates, the absorption factors appearing in Eq. $A_i v_i = -f_i$ May be evaluated for component i on each plate j. Since the matrix is in

tridiagonal form, this matrix equation may be solved for the calculated values of the vapour rates for component i by use of Thomas algorithm.

The procedure proposed by Boston and Sullivan for Thomas algorithm is used here in the following form.

$$
\begin{aligned}
f_1 &= -\frac{1}{M_1} & M_1 &= 1 + A_{1,i} \\
f_2 &= -\frac{M_1}{M_2} & M_2 &= A_{2,i} M_1 + 1 \\
f_k &= -\frac{M_{k-1}}{M_k} & M_k &= A_{k,i} M_{k-1} + 1 \quad , k = 2,3, \ldots\ldots\ldots N-1 \\
g_1 &= g_2 = \cdots\ldots\ldots\ldots = g_{f-1} = 0 \\
g_{f-1} &= v_{f,i} \frac{M_{f-2}}{M_{f-1}} \\
g_f &= (l_{F,i} + A_{f-1,i} g_{f-1}) \frac{M_{f-1}}{M_f} \\
g_k &= A_{k-1} g_{k-1} \frac{M_{k-1}}{M_k} \quad , \; k = f+1, f+2, \ldots\ldots, N
\end{aligned}
\qquad (52)
$$

Again after the f's and g's have been computed, the values of flow rates, are computed by use of the following equations for all components on each plate

$$
\begin{aligned}
x_N &= g_N \\
x_k &= g_k - f_k x_{k+1} \, , \; k = N-1, N-2, \ldots\ldots\ldots, 2, 1
\end{aligned}
\qquad (53)
$$

After the recurrence formulas have been applied for each component i and the set of component vapor rates $(v_{j,i})_{ca}$ have been found, the corresponding set of liquid rates $(l_{j,i})_{ca}$ are then calculated.

These sets of calculated flow rates are used in conjunction with the θ method of the convergence and the K_b method in the determination of an improved set of temperatures.

3. COMPARISION OF RESULTS

The output results of the program TGXBPTH are compared with the results of Hysys in Tables-2-10, since the TGXBPTH program takes less number of iterations when compared to other programs except for the Depropanizer – II and also the θ values are close to the unity than those of other programs. The results of the all the programs are given in the Appendix-III.

Table 2: Comparison of results: Ethane splitter

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions											
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					methane		ethane		propylene		propane		i-butane		n-butane	
0	2757.05	2757.05	2.89	2.89	0.1299	0.1262	0.8700	0.8732	0.0001	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
1	2757.05	2757.05	2.89	2.53	0.0136	0.0186	0.9858	0.9802	0.0004	0.0009	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000
2	2757.78	2757.72	4.00	5.74	0.0050	0.0078	0.9931	0.9884	0.0013	0.0026	0.0006	0.0012	0.0000	0.0000	0.0000	0.0000
3	2758.50	2758.39	4.41	6.28	0.0044	0.0068	0.9898	0.9825	0.0037	0.0068	0.0021	0.0038	0.0000	0.0000	0.0000	0.0000
4	2759.22	2759.05	4.84	7.00	0.0043	0.0067	0.9776	0.9635	0.0106	0.0176	0.0073	0.0119	0.0001	0.0002	0.0001	0.0001
5	2759.94	2759.72	6.11	8.89	0.0043	0.0065	0.9406	0.9129	0.0288	0.0425	0.0242	0.0350	0.0013	0.0018	0.0009	0.0013
6	2760.66	2760.39	10.05	14.08	0.0042	0.0061	0.8353	0.7890	0.0688	0.0888	0.0704	0.0891	0.0106	0.0134	0.0108	0.0136
Feed	2761.39	2761.05	21.75	27.82	0.0039	0.0052	0.5970	0.5475	0.1139	0.1312	0.1408	0.1589	0.0587	0.0640	0.0857	0.0930
8	2762.11	2761.72	24.27	31.12	0.0005	0.0008	0.5877	0.5269	0.1213	0.1444	0.1461	0.1691	0.0588	0.0649	0.0856	0.0939
9	2762.83	2762.39	26.74	34.79	0.0000	0.0001	0.5474	0.4744	0.1412	0.1717	0.1625	0.1914	0.0608	0.0667	0.0880	0.0957
10	2763.55	2763.05	31.88	41.45	0.0000	0.0000	0.4618	0.3795	0.1826	0.2181	0.1985	0.2329	0.0647	0.0702	0.0924	0.0992
11	2764.27	2763.72	41.43	51.54	0.0000	0.0000	0.3258	0.2558	0.2459	0.2728	0.2592	0.2898	0.0707	0.0764	0.0984	0.1051
12	2765.00	2764.39	54.63	62.89	0.0000	0.0000	0.1801	0.1432	0.3022	0.3096	0.3275	0.3425	0.0816	0.0878	0.1085	0.1170
13	2765.72	2765.05	68.16	73.59	0.0000	0.0000	0.0768	0.0668	0.3089	0.3051	0.3637	0.3650	0.1082	0.1128	0.1424	0.1503
14	2765.72	2765.72	88.73	85.65	0.0000	0.0000	0.0244	0.0246	0.2439	0.2438	0.3252	0.3252	0.1626	0.1626	0.2439	0.2439

P.W. – present work

Table 3: Comparison of results: Depropanizer-I

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions									
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					ethane		propane		i-butane		n-butane		n-pentane	
0	2171.85	2171.85	57.22	62.45	0.0145	0.0145	0.9828	0.9832	0.0024	0.0020	0.0003	0.0003	0.0000	0.0000
1	2171.85	2171.85	57.22	62.29	0.0038	0.0043	0.9893	0.9899	0.0059	0.0050	0.0010	0.0008	0.0000	0.0000
2	2172.55	2172.52	61.31	62.71	0.0020	0.0024	0.9842	0.9863	0.0113	0.0093	0.0025	0.0020	0.0000	0.0000
3	2173.25	2173.18	61.72	63.06	0.0017	0.0020	0.9733	0.9778	0.0195	0.0159	0.0056	0.0043	0.0000	0.0000
4	2173.95	2173.85	62.31	63.55	0.0016	0.0019	0.9551	0.9636	0.0315	0.0255	0.0117	0.0090	0.0000	0.0000
5	2174.66	2174.51	63.27	64.32	0.0016	0.0019	0.9261	0.9408	0.0486	0.0393	0.0236	0.0179	0.0001	0.0001
6	2175.36	2175.18	64.78	65.57	0.0016	0.0018	0.8818	0.9052	0.0708	0.0579	0.0453	0.0346	0.0005	0.0004
7	2176.06	2175.85	67.08	67.56	0.0015	0.0018	0.8186	0.8516	0.0962	0.0811	0.0811	0.0634	0.0027	0.0021
8	2176.76	2176.51	70.43	70.69	0.0015	0.0017	0.7353	0.7743	0.1188	0.1056	0.1319	0.1082	0.0125	0.0101
9	2177.46	2177.18	75.37	75.76	0.0014	0.0016	0.6333	0.6679	0.1286	0.1235	0.1871	0.1649	0.0496	0.0422
Feed	2178.16	2177.85	83.06	84.55	0.0013	0.0014	0.5147	0.5279	0.1138	0.1211	0.2150	0.2084	0.1553	0.1412
11	2178.87	2178.51	84.96	87.61	0.0003	0.0004	0.4831	0.4753	0.1305	0.1483	0.2285	0.2316	0.1575	0.1443
12	2179.57	2179.18	87.90	92.21	0.0001	0.0001	0.4307	0.3970	0.1576	0.1869	0.2508	0.2669	0.1608	0.1491
13	2180.27	2179.85	92.28	98.36	0.0000	0.0000	0.3556	0.3007	0.1958	0.2316	0.2840	0.3125	0.1646	0.1551
14	2180.97	2180.51	98.03	105.16	0.0000	0.0000	0.2653	0.2052	0.2405	0.2723	0.3265	0.3611	0.1677	0.1614
15	2181.67	2181.18	104.31	111.34	0.0000	0.0000	0.1767	0.1277	0.2809	0.2999	0.3729	0.4053	0.1695	0.1670
16	2182.37	2181.85	109.96	116.11	0.0000	0.0000	0.1060	0.0742	0.3066	0.3119	0.4168	0.4418	0.1706	0.1721
17	2183.08	2182.51	114.29	119.48	0.0000	0.0000	0.0583	0.0410	0.3137	0.3099	0.4543	0.4709	0.1736	0.1783
18	2183.78	2183.18	117.49	122.00	0.0000	0.0000	0.0301	0.0217	0.3032	0.2957	0.4836	0.4926	0.1831	0.1900
19	2184.48	2183.85	120.36	124.49	0.0000	0.0000	0.0146	0.0110	0.2765	0.2692	0.4994	0.5022	0.2095	0.2176
20	2185.18	2184.51	124.30	128.24	0.0000	0.0000	0.0065	0.0051	0.2317	0.2272	0.4865	0.4850	0.2753	0.2827
21	2185.18	2185.18	137.80	135.07	0.0000	0.0000	0.0025	0.0021	0.1661	0.1665	0.4161	0.4162	0.4153	0.4153

Table 4: Comparison of results: Paraffin separation

Plate number	Pressure (kPa)		Temperature (°C)		Liqud Compositions											
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					nonane		n-decane		undecane		n-dodacane		n-tridecane		n-tetradecane	
0	70.66	70.66	161.54	166.54	0.1318	0.1414	0.5689	0.5963	0.2571	0.2429	0.0419	0.0193	0.0003	0.0001	0.0000	0.0000
1	70.66	70.66	167.97	166.02	0.0592	0.0665	0.4621	0.5093	0.3728	0.3717	0.1045	0.0520	0.0014	0.0005	0.0000	0.0000
2	71.39	71.33	171.89	169.47	0.0396	0.0454	0.3825	0.4351	0.4117	0.4304	0.1627	0.0877	0.0035	0.0014	0.0000	0.0000
3	72.13	71.99	174.34	171.71	0.0342	0.0391	0.3358	0.3866	0.4111	0.4469	0.2119	0.1244	0.0070	0.0030	0.0000	0.0000
4	72.86	72.66	176.09	173.40	0.0323	0.0366	0.3095	0.3561	0.3948	0.4409	0.2504	0.1602	0.0128	0.0060	0.0001	0.0001
5	73.59	73.33	177.48	174.85	0.0313	0.0352	0.2940	0.3356	0.3742	0.4238	0.2781	0.1936	0.0220	0.0115	0.0004	0.0004
6	74.33	73.99	178.73	176.24	0.0307	0.0342	0.2834	0.3200	0.3537	0.4014	0.2948	0.2224	0.0362	0.0209	0.0012	0.0011
7	75.06	74.66	179.99	177.68	0.0301	0.0332	0.2748	0.3062	0.3341	0.3764	0.3003	0.2443	0.0570	0.0366	0.0036	0.0033
8	75.79	75.33	181.41	179.33	0.0295	0.0320	0.2663	0.2921	0.3144	0.3492	0.2940	0.2562	0.0858	0.0611	0.0100	0.0093
9	76.53	75.99	183.18	181.44	0.0287	0.0306	0.2560	0.2755	0.2929	0.3184	0.2745	0.2544	0.1215	0.0963	0.0262	0.0248
10	77.26	76.66	185.59	184.35	0.0277	0.0287	0.2427	0.2541	0.2675	0.2820	0.2411	0.2346	0.1585	0.1402	0.0625	0.0604
Feed	77.99	77.33	188.90	188.46	0.0262	0.0262	0.2254	0.2267	0.2373	0.2393	0.1956	0.1959	0.1840	0.1819	0.1315	0.1300
12	78.73	77.99	189.19	188.81	0.0265	0.0261	0.2260	0.2267	0.2373	0.2393	0.1954	0.1959	0.1836	0.1819	0.1312	0.1301
13	79.46	78.66	189.49	189.16	0.0268	0.0261	0.2267	0.2266	0.2373	0.2393	0.1951	0.1960	0.1832	0.1819	0.1309	0.1301
14	80.19	79.33	189.79	189.51	0.0271	0.0260	0.2273	0.2266	0.2373	0.2394	0.1949	0.1960	0.1829	0.1819	0.1305	0.1301
15	80.93	79.99	190.09	189.86	0.0273	0.0259	0.2280	0.2266	0.2373	0.2394	0.1946	0.1960	0.1825	0.1820	0.1302	0.1301
16	81.66	80.66	190.39	190.22	0.0275	0.0257	0.2288	0.2267	0.2374	0.2395	0.1944	0.1961	0.1821	0.1820	0.1299	0.1301
17	82.39	81.33	190.70	190.58	0.0274	0.0254	0.2296	0.2267	0.2375	0.2396	0.1942	0.1961	0.1818	0.1820	0.1296	0.1301
18	83.13	81.99	191.03	190.96	0.0271	0.0248	0.2305	0.2268	0.2377	0.2398	0.1940	0.1962	0.1814	0.1821	0.1293	0.1302
19	83.86	82.66	191.41	191.38	0.0263	0.0239	0.2312	0.2267	0.2383	0.2404	0.1940	0.1965	0.1811	0.1822	0.1290	0.1302
20	84.59	83.33	191.94	191.93	0.0246	0.0223	0.2307	0.2254	0.2399	0.2417	0.1948	0.1974	0.1813	0.1828	0.1288	0.1304
21	85.33	83.99	193.02	192.97	0.0211	0.0192	0.2233	0.2180	0.2425	0.2438	0.1986	0.2011	0.1843	0.1858	0.1301	0.1321
22	85.33	84.66	196.58	196.60	0.0142	0.0132	0.1857	0.1826	0.2325	0.2342	0.2087	0.2112	0.2066	0.2067	0.1522	0.1522

Table 5: Comparison of results: Depropanizer-II

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions											
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					methane		ethane		propane		n-butane		n-pentane		n-hexane	
0	2171.25	2171.25	28.14	28.21	0.4341	0.4341	0.1503	0.1503	0.4157	0.4157	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	2171.25	2171.25	26.98	28.05	0.0252	0.0366	0.0745	0.0789	0.9002	0.8845	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	2171.84	2171.78	47.80	47.64	0.0081	0.0136	0.0339	0.0400	0.9580	0.9463	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
3	2172.43	2172.31	50.55	49.57	0.0068	0.0125	0.0229	0.0304	0.9702	0.9569	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
4	2173.03	2172.85	51.06	49.89	0.0066	0.0124	0.0203	0.0281	0.9729	0.9588	0.0002	0.0007	0.0000	0.0000	0.0000	0.0000
5	2173.62	2173.38	51.19	50.00	0.0066	0.0124	0.0197	0.0276	0.9731	0.9583	0.0006	0.0017	0.0000	0.0000	0.0000	0.0000
6	2174.21	2173.91	51.26	50.12	0.0066	0.0123	0.0195	0.0274	0.9722	0.9556	0.0017	0.0046	0.0000	0.0000	0.0000	0.0000
7	2174.80	2174.45	51.38	50.41	0.0066	0.0123	0.0195	0.0273	0.9690	0.9481	0.0049	0.0121	0.0001	0.0002	0.0000	0.0000
8	2175.40	2174.98	51.69	51.15	0.0066	0.0122	0.0194	0.0269	0.9596	0.9280	0.0136	0.0311	0.0007	0.0016	0.0001	0.0002
9	2175.99	2175.51	52.73	53.43	0.0065	0.0120	0.0191	0.0259	0.9294	0.8707	0.0370	0.0754	0.0059	0.0117	0.0021	0.0042
Feed	2176.58	2176.05	57.85	62.74	0.0065	0.0111	0.0180	0.0223	0.8051	0.6887	0.0866	0.1458	0.0415	0.0660	0.0423	0.0662
11	2177.17	2176.58	67.54	75.59	0.0003	0.0008	0.0049	0.0069	0.8218	0.6869	0.0947	0.1714	0.0391	0.0672	0.0393	0.0667
12	2177.77	2177.11	69.95	80.02	0.0000	0.0001	0.0013	0.0020	0.7905	0.6338	0.1275	0.2270	0.0405	0.0696	0.0402	0.0675
13	2178.36	2177.65	73.92	86.54	0.0000	0.0000	0.0003	0.0005	0.7058	0.5233	0.2071	0.3329	0.0442	0.0742	0.0425	0.0691
14	2178.95	2178.18	81.97	96.81	0.0000	0.0000	0.0001	0.0001	0.5455	0.3657	0.3587	0.4814	0.0500	0.0813	0.0458	0.0714
15	2179.54	2178.71	94.37	108.69	0.0000	0.0000	0.0000	0.0000	0.3401	0.2133	0.5549	0.6225	0.0571	0.0903	0.0479	0.0739
16	2180.14	2179.25	107.31	118.54	0.0000	0.0000	0.0000	0.0000	0.1708	0.1079	0.7141	0.7138	0.0668	0.1019	0.0484	0.0763
17	2180.73	2179.78	116.89	125.25	0.0000	0.0000	0.0000	0.0000	0.0731	0.0497	0.7887	0.7483	0.0871	0.1215	0.0511	0.0805
18	2181.32	2180.31	123.82	130.57	0.0000	0.0000	0.0000	0.0000	0.0280	0.0212	0.7743	0.7252	0.1307	0.1588	0.0670	0.0947
19	2181.91	2180.85	132.31	138.00	0.0000	0.0000	0.0000	0.0000	0.0094	0.0081	0.6562	0.6239	0.2054	0.2198	0.1290	0.1481
20	2181.91	2181.38	148.16	152.57	0.0000	0.0000	0.0000	0.0000	0.0025	0.0025	0.4239	0.4239	0.2743	0.2743	0.2993	0.2993

Table 6: Comparison of results: Xylene fractionation

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions							
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					ethylbenzene		p-xylene		m-xylene		o-xylene	
0	101.33	101.33	138.59	138.52	0.0609	0.0610	0.6883	0.6888	0.2314	0.2315	0.0194	0.0188
1	101.33	101.33	138.61	138.67	0.0571	0.0573	0.6859	0.6856	0.2343	0.2351	0.0227	0.0220
2	101.72	101.72	138.80	138.85	0.0538	0.0541	0.6832	0.6822	0.2367	0.2383	0.0263	0.0254
3	102.12	102.12	138.98	139.02	0.0510	0.0513	0.6802	0.6786	0.2388	0.2410	0.0301	0.0291
4	102.52	102.52	139.16	139.20	0.0485	0.0489	0.6770	0.6748	0.2405	0.2434	0.0341	0.0329
5	102.92	102.92	139.34	139.37	0.0463	0.0468	0.6735	0.6708	0.2419	0.2453	0.0383	0.0370
6	103.32	103.32	139.52	139.55	0.0444	0.0450	0.6699	0.6667	0.2429	0.2470	0.0428	0.0413
7	103.72	103.72	139.70	139.72	0.0428	0.0434	0.6660	0.6625	0.2437	0.2483	0.0475	0.0459
8	104.12	104.12	139.88	139.90	0.0414	0.0420	0.6620	0.6581	0.2442	0.2492	0.0524	0.0507
9	104.52	104.52	140.06	140.07	0.0401	0.0408	0.6578	0.6536	0.2444	0.2499	0.0577	0.0557
10	104.92	104.92	140.24	140.25	0.0390	0.0397	0.6535	0.6489	0.2443	0.2503	0.0632	0.0610
11	105.32	105.32	140.42	140.43	0.0381	0.0388	0.6490	0.6442	0.2441	0.2505	0.0689	0.0666
12	105.72	105.72	140.61	140.61	0.0372	0.0379	0.6443	0.6393	0.2436	0.2504	0.0749	0.0724
13	106.12	106.12	140.79	140.79	0.0364	0.0372	0.6395	0.6343	0.2429	0.2500	0.0812	0.0785
14	106.52	106.52	140.97	140.96	0.0358	0.0365	0.6345	0.6292	0.2420	0.2495	0.0878	0.0848
15	106.92	106.92	141.16	141.14	0.0351	0.0359	0.6294	0.6240	0.2409	0.2487	0.0946	0.0914
16	107.32	107.32	141.35	141.33	0.0346	0.0353	0.6241	0.6187	0.2396	0.2477	0.1017	0.0983
17	107.72	107.72	141.53	141.51	0.0341	0.0348	0.6188	0.6133	0.2382	0.2465	0.1090	0.1054
18	108.12	108.12	141.72	141.69	0.0336	0.0344	0.6132	0.6077	0.2366	0.2452	0.1165	0.1127
19	108.52	108.52	141.91	141.87	0.0332	0.0340	0.6076	0.6021	0.2349	0.2437	0.1243	0.1203
20	108.92	108.92	142.10	142.06	0.0328	0.0336	0.6019	0.5964	0.2330	0.2420	0.1323	0.1281
21	109.32	109.32	142.29	142.24	0.0324	0.0332	0.5960	0.5905	0.2310	0.2402	0.1405	0.1361
22	109.72	109.72	142.48	142.43	0.0321	0.0328	0.5901	0.5847	0.2289	0.2383	0.1489	0.1442
23	110.12	110.12	142.67	142.61	0.0317	0.0325	0.5841	0.5787	0.2267	0.2362	0.1575	0.1526
24	110.52	110.52	142.86	142.80	0.0314	0.0322	0.5780	0.5727	0.2245	0.2340	0.1662	0.1611

Table 6: Comparison of results: Xylene fractionation (Contd.....)

25	110.92	110.92	143.06	142.99	0.0311	0.0319	0.5718	0.5666	0.2221	0.2318	0.1750	0.1698
26	111.32	111.32	143.25	143.18	0.0308	0.0316	0.5656	0.5605	0.2197	0.2294	0.1840	0.1785
27	111.72	111.72	143.44	143.36	0.0305	0.0313	0.5594	0.5544	0.2172	0.2270	0.1930	0.1874
28	112.12	112.12	143.63	143.55	0.0302	0.0310	0.5531	0.5482	0.2146	0.2245	0.2020	0.1963
29	112.52	112.52	143.83	143.74	0.0299	0.0307	0.5469	0.5421	0.2121	0.2219	0.2111	0.2053
30	112.92	112.92	144.02	143.92	0.0297	0.0304	0.5406	0.5359	0.2095	0.2193	0.2202	0.2143
31	113.32	113.32	144.21	144.11	0.0294	0.0302	0.5344	0.5298	0.2069	0.2167	0.2293	0.2233
32	113.72	113.72	144.40	144.30	0.0292	0.0299	0.5283	0.5238	0.2042	0.2141	0.2383	0.2322
33	114.12	114.12	144.59	144.48	0.0289	0.0297	0.5222	0.5178	0.2016	0.2114	0.2473	0.2411
34	114.52	114.52	144.78	144.67	0.0287	0.0294	0.5162	0.5118	0.1990	0.2088	0.2561	0.2499
35	114.92	114.92	144.97	144.85	0.0284	0.0292	0.5103	0.5060	0.1965	0.2062	0.2648	0.2586
36	115.32	115.32	145.15	145.04	0.0282	0.0290	0.5045	0.5003	0.1939	0.2035	0.2734	0.2672
37	115.72	115.72	145.34	145.22	0.0280	0.0287	0.4988	0.4946	0.1914	0.2010	0.2818	0.2757
38	116.12	116.12	145.52	145.40	0.0278	0.0285	0.4932	0.4891	0.1890	0.1984	0.2901	0.2840
39	116.52	116.52	145.71	145.58	0.0275	0.0283	0.4878	0.4837	0.1866	0.1959	0.2981	0.2921
40	116.92	116.92	145.89	145.75	0.0273	0.0281	0.4825	0.4785	0.1842	0.1934	0.3060	0.3000
41	117.32	117.32	146.07	145.93	0.0271	0.0279	0.4774	0.4734	0.1819	0.1911	0.3136	0.3077
42	117.72	117.72	146.24	146.11	0.0270	0.0277	0.4724	0.4685	0.1797	0.1887	0.3209	0.3151
43	118.12	118.12	146.42	146.28	0.0268	0.0275	0.4676	0.4637	0.1776	0.1864	0.3281	0.3224
44	118.52	118.52	146.59	146.45	0.0266	0.0273	0.4630	0.4591	0.1755	0.1842	0.3349	0.3294
45	118.92	118.92	146.77	146.62	0.0264	0.0272	0.4586	0.4546	0.1735	0.1821	0.3415	0.3361
Feed	119.32	119.32	146.94	146.79	0.0263	0.0270	0.4543	0.4504	0.1715	0.1801	0.3479	0.3426
47	119.72	119.72	147.21	147.06	0.0238	0.0246	0.4380	0.4336	0.1674	0.1766	0.3708	0.3652
48	120.12	120.12	147.49	147.33	0.0215	0.0223	0.4207	0.4159	0.1627	0.1726	0.3951	0.3892
49	120.52	120.52	147.78	147.62	0.0194	0.0202	0.4026	0.3974	0.1575	0.1680	0.4206	0.4144
50	120.92	120.92	148.07	147.91	0.0174	0.0182	0.3837	0.3782	0.1519	0.1628	0.4471	0.4408
51	121.32	121.32	148.37	148.20	0.0155	0.0163	0.3641	0.3584	0.1458	0.1571	0.4746	0.4682
52	121.72	121.72	148.68	148.50	0.0138	0.0145	0.3441	0.3382	0.1394	0.1510	0.5027	0.4962

Table 6: Comparison of results: Xylene fractionation (Contd.....)

53	122.12	122.12	148.98	148.80	0.0122	0.0129	0.3239	0.3177	0.1326	0.1445	0.5313	0.5249
54	122.52	122.52	149.29	149.11	0.0107	0.0114	0.3035	0.2972	0.1256	0.1376	0.5602	0.5538
55	122.92	122.92	149.59	149.41	0.0094	0.0101	0.2831	0.2768	0.1185	0.1305	0.5889	0.5827
56	123.32	123.32	149.90	149.72	0.0082	0.0088	0.2630	0.2566	0.1113	0.1232	0.6175	0.6114
57	123.72	123.72	150.20	150.02	0.0072	0.0077	0.2433	0.2369	0.1041	0.1158	0.6454	0.6396
58	124.12	124.12	150.50	150.31	0.0062	0.0067	0.2242	0.2177	0.0969	0.1083	0.6727	0.6672
59	124.52	124.52	150.79	150.60	0.0054	0.0058	0.2058	0.1994	0.0898	0.1010	0.6990	0.6938
60	124.92	124.92	151.07	150.89	0.0046	0.0050	0.1881	0.1818	0.0830	0.0937	0.7243	0.7194
61	125.32	125.32	151.35	151.17	0.0039	0.0043	0.1714	0.1652	0.0764	0.0867	0.7483	0.7438
62	125.72	125.72	151.62	151.43	0.0034	0.0037	0.1556	0.1495	0.0700	0.0799	0.7710	0.7669
63	126.12	126.12	151.88	151.69	0.0029	0.0032	0.1409	0.1349	0.0640	0.0734	0.7922	0.7885
64	126.52	126.52	152.13	151.95	0.0024	0.0027	0.1271	0.1214	0.0583	0.0672	0.8121	0.8087
65	126.92	126.92	152.37	152.19	0.0021	0.0023	0.1144	0.1089	0.0530	0.0613	0.8305	0.8275
66	127.32	127.32	152.60	152.42	0.0017	0.0019	0.1027	0.0974	0.0481	0.0558	0.8475	0.8448
67	127.72	127.72	152.83	152.64	0.0015	0.0016	0.0920	0.0870	0.0434	0.0507	0.8631	0.8607
68	128.12	128.12	153.04	152.86	0.0012	0.0014	0.0822	0.0774	0.0392	0.0459	0.8774	0.8752
69	128.52	128.52	153.25	153.07	0.0010	0.0012	0.0733	0.0688	0.0353	0.0415	0.8903	0.8885
70	128.92	128.92	153.45	153.26	0.0009	0.0010	0.0653	0.0610	0.0317	0.0375	0.9021	0.9005
71	129.32	129.32	153.64	153.46	0.0007	0.0008	0.0581	0.0541	0.0284	0.0338	0.9128	0.9113
72	129.72	129.72	153.83	153.64	0.0006	0.0007	0.0515	0.0478	0.0255	0.0304	0.9224	0.9211
73	130.12	130.12	154.01	153.82	0.0005	0.0006	0.0457	0.0422	0.0228	0.0273	0.9310	0.9299
74	130.52	130.52	154.18	153.99	0.0004	0.0005	0.0405	0.0372	0.0204	0.0245	0.9387	0.9378
75	130.92	130.92	154.35	154.16	0.0003	0.0004	0.0358	0.0328	0.0182	0.0220	0.9457	0.9448
76	131.32	131.32	154.51	154.32	0.0003	0.0003	0.0317	0.0289	0.0162	0.0197	0.9518	0.9511
77	131.72	131.72	154.67	154.47	0.0002	0.0003	0.0280	0.0254	0.0144	0.0176	0.9574	0.9567
78	132.12	132.12	154.83	154.63	0.0002	0.0002	0.0247	0.0223	0.0129	0.0157	0.9623	0.9617
79	132.52	132.52	154.98	154.78	0.0002	0.0002	0.0218	0.0196	0.0114	0.0140	0.9666	0.9662
80	132.92	132.92	155.12	154.92	0.0001	0.0002	0.0192	0.0172	0.0102	0.0125	0.9705	0.9701

Table 6: Comparison of results: Xylene fractionation (Contd.....)

81	133.32	133.32	155.27	155.06	0.0001	0.0001	0.0169	0.0151	0.0090	0.0112	0.9740	0.9736
82	133.72	133.72	155.41	155.20	0.0001	0.0001	0.0149	0.0132	0.0080	0.0099	0.9770	0.9767
83	134.12	134.12	155.55	155.34	0.0001	0.0001	0.0131	0.0116	0.0071	0.0089	0.9797	0.9795
84	134.52	134.52	155.69	155.48	0.0001	0.0001	0.0115	0.0101	0.0063	0.0079	0.9821	0.9819
85	134.92	134.92	155.82	155.61	0.0001	0.0001	0.0101	0.0089	0.0056	0.0070	0.9842	0.9840
86	135.32	135.32	155.95	155.74	0.0000	0.0001	0.0089	0.0078	0.0049	0.0062	0.9861	0.9859
87	135.72	135.72	156.08	155.87	0.0000	0.0000	0.0078	0.0068	0.0044	0.0055	0.9878	0.9876
88	136.12	136.12	156.21	156.00	0.0000	0.0000	0.0069	0.0059	0.0039	0.0049	0.9892	0.9891
89	136.52	136.52	156.34	156.12	0.0000	0.0000	0.0060	0.0052	0.0034	0.0044	0.9905	0.9904
90	136.92	136.92	156.47	156.25	0.0000	0.0000	0.0053	0.0045	0.0030	0.0039	0.9917	0.9916
91	137.32	137.32	156.60	156.37	0.0000	0.0000	0.0046	0.0039	0.0027	0.0034	0.9927	0.9926
92	137.72	137.72	156.72	156.49	0.0000	0.0000	0.0040	0.0034	0.0024	0.0030	0.9936	0.9935
93	138.12	138.12	156.85	156.62	0.0000	0.0000	0.0035	0.0030	0.0021	0.0027	0.9944	0.9943
94	138.52	138.52	156.97	156.74	0.0000	0.0000	0.0031	0.0026	0.0018	0.0024	0.9951	0.9950
95	138.92	138.92	157.09	156.86	0.0000	0.0000	0.0027	0.0023	0.0016	0.0021	0.9957	0.9956
96	139.32	139.32	157.21	156.98	0.0000	0.0000	0.0024	0.0020	0.0014	0.0019	0.9962	0.9962
97	139.72	139.72	157.33	157.10	0.0000	0.0000	0.0021	0.0017	0.0012	0.0016	0.9967	0.9967
98	140.12	140.12	157.46	157.21	0.0000	0.0000	0.0018	0.0015	0.0011	0.0014	0.9971	0.9971
99	140.52	140.52	157.57	157.33	0.0000	0.0000	0.0015	0.0013	0.0009	0.0013	0.9975	0.9975
100	140.92	140.92	157.58	157.45	0.0000	0.0000	0.0013	0.0011	0.0008	0.0011	0.9978	0.9978

Table 7: Comparison of results: Ethylbenzene – Styrene separation

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions							
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					toluene		ethyl Benzene		styrene		cumene	
0	6.67	6.67	56.94	56.13	0.0220	0.0220	0.9640	0.9625	0.0140	0.0155	0.0000	0.0000
1	6.67	6.67	57.43	56.13	0.0088	0.0087	0.9710	0.9697	0.0202	0.0216	0.0000	0.0000
2	7.07	7.07	58.98	57.72	0.0042	0.0041	0.9680	0.9664	0.0278	0.0295	0.0000	0.0000
3	7.48	7.47	60.37	59.15	0.0025	0.0025	0.9605	0.9584	0.0370	0.0391	0.0000	0.0000
4	7.89	7.87	61.68	60.50	0.0020	0.0019	0.9500	0.9474	0.0480	0.0506	0.0000	0.0001
5	8.30	8.27	62.95	61.79	0.0018	0.0018	0.9370	0.9340	0.0612	0.0642	0.0000	0.0001
6	8.70	8.67	64.18	63.05	0.0017	0.0017	0.9215	0.9180	0.0768	0.0802	0.0000	0.0001
7	9.11	9.07	65.39	64.29	0.0017	0.0017	0.9033	0.8994	0.0949	0.0988	0.0001	0.0002
8	9.52	9.47	66.58	65.50	0.0017	0.0017	0.8824	0.8780	0.1158	0.1201	0.0001	0.0002
9	9.93	9.87	67.75	66.69	0.0017	0.0017	0.8586	0.8539	0.1395	0.1441	0.0002	0.0003
10	10.34	10.27	68.91	67.87	0.0017	0.0017	0.8321	0.8272	0.1659	0.1707	0.0002	0.0004
11	10.74	10.67	70.06	69.04	0.0017	0.0016	0.8032	0.7981	0.1948	0.1997	0.0004	0.0006
12	11.15	11.07	71.20	70.19	0.0017	0.0016	0.7721	0.7670	0.2257	0.2305	0.0005	0.0008
13	11.56	11.47	72.33	71.33	0.0016	0.0016	0.7395	0.7345	0.2581	0.2628	0.0007	0.0011
14	11.97	11.87	73.44	72.45	0.0016	0.0016	0.7060	0.7013	0.2913	0.2957	0.0011	0.0014
15	12.37	12.27	74.54	73.55	0.0016	0.0016	0.6723	0.6680	0.3246	0.3286	0.0015	0.0018
Feed	12.78	12.67	75.61	74.63	0.0016	0.0016	0.6391	0.6354	0.3572	0.3608	0.0020	0.0023
17	13.19	13.07	76.44	75.48	0.0007	0.0007	0.6390	0.6347	0.3583	0.3623	0.0020	0.0023
18	13.60	13.47	77.24	76.29	0.0003	0.0003	0.6384	0.6336	0.3593	0.3638	0.0020	0.0023
19	14.00	13.87	78.00	77.07	0.0001	0.0001	0.6376	0.6323	0.3602	0.3653	0.0021	0.0023
20	14.41	14.27	78.75	77.83	0.0001	0.0001	0.6366	0.6308	0.3613	0.3668	0.0021	0.0023
21	14.82	14.67	79.48	78.57	0.0000	0.0000	0.6355	0.6292	0.3624	0.3684	0.0021	0.0023
22	15.23	15.07	80.19	79.29	0.0000	0.0000	0.6343	0.6275	0.3636	0.3701	0.0021	0.0023
23	15.63	15.47	80.89	80.00	0.0000	0.0000	0.6329	0.6256	0.3650	0.3720	0.0021	0.0023
24	16.04	15.87	81.57	80.70	0.0000	0.0000	0.6313	0.6235	0.3666	0.3741	0.0021	0.0024
25	16.45	16.27	82.24	81.38	0.0000	0.0000	0.6295	0.6212	0.3685	0.3765	0.0021	0.0024

Table 7: Comparison of results: Ethylbenzene – Styrene separation (Contd....)

26	16.86	16.67	82.91	82.06	0.0000	0.0000	0.6273	0.6185	0.3707	0.3791	0.0021	0.0024
27	17.27	17.07	83.56	82.72	0.0000	0.0000	0.6247	0.6154	0.3732	0.3822	0.0021	0.0024
28	17.67	17.47	84.20	83.37	0.0000	0.0000	0.6216	0.6119	0.3763	0.3858	0.0021	0.0024
29	18.08	17.87	84.84	84.02	0.0000	0.0000	0.6179	0.6077	0.3800	0.3899	0.0021	0.0024
30	18.49	18.27	85.47	84.66	0.0000	0.0000	0.6135	0.6029	0.3844	0.3947	0.0021	0.0024
31	18.90	18.67	86.10	85.30	0.0000	0.0000	0.6082	0.5972	0.3897	0.4004	0.0021	0.0024
32	19.30	19.07	86.73	85.93	0.0000	0.0000	0.6018	0.5905	0.3961	0.4071	0.0021	0.0025
33	19.71	19.47	87.36	86.57	0.0000	0.0000	0.5941	0.5825	0.4038	0.4150	0.0021	0.0025
34	20.12	19.87	87.99	87.21	0.0000	0.0000	0.5849	0.5732	0.4129	0.4243	0.0021	0.0025
35	20.53	20.27	88.63	87.85	0.0000	0.0000	0.5740	0.5623	0.4238	0.4352	0.0022	0.0025
36	20.93	20.66	89.27	88.49	0.0000	0.0000	0.5611	0.5495	0.4367	0.4479	0.0022	0.0026
37	21.34	21.06	89.93	89.15	0.0000	0.0000	0.5460	0.5347	0.4518	0.4627	0.0022	0.0026
38	21.75	21.46	90.59	89.82	0.0000	0.0000	0.5285	0.5176	0.4692	0.4797	0.0023	0.0027
39	22.16	21.86	91.28	90.50	0.0000	0.0000	0.5084	0.4981	0.4893	0.4992	0.0023	0.0027
40	22.56	22.26	91.97	91.19	0.0000	0.0000	0.4857	0.4761	0.5120	0.5211	0.0023	0.0028
41	22.97	22.66	92.69	91.90	0.0000	0.0000	0.4603	0.4516	0.5373	0.5456	0.0024	0.0029
42	23.38	23.06	93.42	92.62	0.0000	0.0000	0.4324	0.4247	0.5652	0.5724	0.0025	0.0029
43	23.79	23.46	94.16	93.36	0.0000	0.0000	0.4022	0.3956	0.5952	0.6014	0.0025	0.0031
44	24.20	23.86	94.92	94.10	0.0000	0.0000	0.3702	0.3647	0.6271	0.6321	0.0026	0.0032
45	24.60	24.26	95.68	94.86	0.0000	0.0000	0.3370	0.3325	0.6603	0.6642	0.0027	0.0033
46	25.01	24.66	96.45	95.62	0.0000	0.0000	0.3030	0.2996	0.6941	0.6969	0.0029	0.0035
47	25.42	25.06	97.21	96.37	0.0000	0.0000	0.2690	0.2666	0.7279	0.7297	0.0031	0.0037
48	25.83	25.46	97.97	97.12	0.0000	0.0000	0.2357	0.2341	0.7610	0.7619	0.0033	0.0040
49	26.23	25.86	98.71	97.85	0.0000	0.0000	0.2037	0.2028	0.7927	0.7928	0.0036	0.0043
50	26.64	26.26	99.43	98.57	0.0000	0.0000	0.1735	0.1732	0.8225	0.8220	0.0040	0.0048
51	27.05	26.66	100.13	99.26	0.0000	0.0000	0.1455	0.1456	0.8499	0.8491	0.0046	0.0053
52	27.46	27.06	100.81	99.94	0.0000	0.0000	0.1199	0.1203	0.8747	0.8737	0.0054	0.0060
53	27.86	27.46	101.46	100.58	0.0000	0.0000	0.0969	0.0974	0.8966	0.8957	0.0065	0.0069
54	27.86	27.86	101.66	101.20	0.0000	0.0000	0.0764	0.0770	0.9156	0.9150	0.0080	0.0080

Table 8: Comparison of results: Biphenyl separation

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions					
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					benzene		toluene		biphenyl	
0	149.59	149.59	93.06	95.79	0.9505	0.9505	0.0495	0.0495	0.0000	0.0000
1	149.59	149.59	94.64	95.67	0.8822	0.8864	0.1178	0.1136	0.0000	0.0000
2	150.16	150.12	96.49	97.31	0.8119	0.8214	0.1881	0.1786	0.0000	0.0001
3	150.74	150.65	98.27	98.91	0.7475	0.7610	0.2525	0.2386	0.0000	0.0005
4	151.31	151.19	99.84	100.43	0.6941	0.7079	0.3057	0.2888	0.0002	0.0033
Feed	151.88	151.72	101.87	102.26	0.6408	0.6553	0.3375	0.3221	0.0217	0.0226
6	152.46	152.25	108.67	108.38	0.4291	0.4521	0.5488	0.5248	0.0221	0.0231
7	153.03	152.79	115.73	115.02	0.2429	0.2647	0.7349	0.7117	0.0222	0.0236
8	153.61	153.32	121.03	120.29	0.1219	0.1368	0.8559	0.8391	0.0222	0.0241
9	154.18	153.85	124.17	123.60	0.0571	0.0656	0.9208	0.9091	0.0221	0.0253
10	154.76	154.39	125.83	125.62	0.0259	0.0301	0.9520	0.9377	0.0221	0.0322
11	155.33	154.92	126.69	128.03	0.0116	0.0131	0.9664	0.9120	0.0221	0.0749
12	155.91	155.45	127.24	136.57	0.0051	0.0047	0.9706	0.7187	0.0243	0.2765
13	156.48	155.99	132.18	161.91	0.0020	0.0010	0.8637	0.3188	0.1343	0.6802
14	157.05	156.52	193.78	190.35	0.0003	0.0001	0.2088	0.0807	0.7909	0.9191
15	157.05	157.05	202.33	202.09	0.0000	0.0000	0.0166	0.0166	0.9834	0.9834

Table 9: Comparison of results: separation of Toluene – Ethylbenzene

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions							
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					benzene		toluene		ethyl benzene		styrene	
0	21.33	21.33	51.50	63.99	0.3657	0.3647	0.4697	0.4857	0.1395	0.1270	0.0252	0.0227
1	21.33	21.33	64.29	63.29	0.1238	0.1305	0.4577	0.4834	0.3333	0.3088	0.0852	0.0773
2	21.78	21.73	74.35	73.04	0.0421	0.0458	0.3149	0.3402	0.4778	0.4587	0.1652	0.1553
3	22.23	22.13	80.41	79.31	0.0219	0.0232	0.1949	0.2107	0.5364	0.5278	0.2468	0.2383
4	22.68	22.53	83.98	83.12	0.0171	0.0173	0.1269	0.1344	0.5331	0.5313	0.3229	0.3170
5	23.13	22.93	86.22	85.49	0.0156	0.0155	0.0938	0.0964	0.4975	0.4984	0.3930	0.3896
Feed	23.58	23.33	87.79	87.13	0.0150	0.0148	0.0784	0.0786	0.4489	0.4499	0.4577	0.4567
7	24.03	23.73	88.98	88.26	0.0103	0.0101	0.0780	0.0775	0.4520	0.4531	0.4597	0.4593
8	24.48	24.13	90.14	89.36	0.0066	0.0065	0.0750	0.0739	0.4555	0.4565	0.4629	0.4631
9	24.93	24.53	91.37	90.54	0.0038	0.0038	0.0672	0.0658	0.4582	0.4591	0.4708	0.4713
10	24.93	24.93	92.46	92.05	0.0017	0.0017	0.0506	0.0496	0.4514	0.4522	0.4963	0.4965

Table 10: Comparison of results: Phenol – Cresol separation

Plate number	Pressure (kPa)		Temperature (°C)		Liquid Compositions							
	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.	Hysys	P.W.
					phenol		o-cresol		m-cresol		2,3-xylenol	
0	20.00	20.00	131.33	131.68	0.9582	0.9555	0.0418	0.0444	0.0000	0.0000	0.0000	0.0000
1	20.00	20.00	131.40	131.68	0.9468	0.9436	0.0532	0.0563	0.0001	0.0001	0.0000	0.0000
2	20.55	20.53	132.21	132.47	0.9337	0.9301	0.0662	0.0698	0.0001	0.0001	0.0000	0.0000
3	21.11	21.06	133.03	133.26	0.9189	0.9148	0.0809	0.0850	0.0002	0.0002	0.0000	0.0000
4	21.66	21.60	133.84	134.04	0.9022	0.8977	0.0974	0.1019	0.0003	0.0004	0.0000	0.0000
5	22.22	22.13	134.65	134.83	0.8836	0.8787	0.1158	0.1206	0.0006	0.0007	0.0000	0.0000
6	22.78	22.66	135.46	135.62	0.8628	0.8577	0.1361	0.1411	0.0010	0.0012	0.0000	0.0000
7	23.33	23.20	136.28	136.41	0.8399	0.8346	0.1583	0.1634	0.0018	0.0020	0.0000	0.0000
8	23.89	23.73	137.10	137.21	0.8148	0.8094	0.1821	0.1871	0.0030	0.0034	0.0000	0.0000
9	24.44	24.26	137.94	138.02	0.7875	0.7821	0.2073	0.2122	0.0051	0.0056	0.0001	0.0001
10	25.00	24.80	138.79	138.85	0.7577	0.7526	0.2335	0.2379	0.0086	0.0093	0.0002	0.0002
11	25.55	25.33	139.68	139.71	0.7254	0.7207	0.2600	0.2638	0.0141	0.0151	0.0005	0.0005
12	26.11	25.86	140.60	140.61	0.6902	0.6859	0.2857	0.2886	0.0230	0.0242	0.0012	0.0013
13	26.66	26.40	141.61	141.59	0.6513	0.6477	0.3090	0.3110	0.0367	0.0383	0.0030	0.0030
14	27.22	26.93	142.73	142.69	0.6077	0.6049	0.3276	0.3285	0.0576	0.0594	0.0071	0.0072
15	27.78	27.46	144.06	143.98	0.5577	0.5558	0.3383	0.3381	0.0876	0.0895	0.0164	0.0165
16	28.33	28.00	145.72	145.60	0.4994	0.4985	0.3363	0.3354	0.1281	0.1297	0.0363	0.0363
Feed	28.89	28.53	147.86	147.71	0.4313	0.4314	0.3168	0.3156	0.1766	0.1777	0.0753	0.0753
18	29.44	29.06	148.87	148.69	0.3941	0.3948	0.3405	0.3387	0.1887	0.1897	0.0767	0.0767
19	30.00	29.60	149.96	149.76	0.3531	0.3545	0.3623	0.3599	0.2059	0.2067	0.0788	0.0789
20	30.55	30.13	151.18	150.95	0.3087	0.3108	0.3792	0.3765	0.2299	0.2304	0.0822	0.0823
21	31.11	30.66	152.56	152.30	0.2618	0.2645	0.3879	0.3850	0.2622	0.2624	0.0881	0.0882
22	31.66	31.20	154.15	153.86	0.2136	0.2166	0.3841	0.3813	0.3034	0.3033	0.0989	0.0989
23	32.22	31.73	156.01	155.69	0.1660	0.1689	0.3642	0.3617	0.3515	0.3511	0.1183	0.1183
24	32.78	32.26	158.20	157.87	0.1211	0.1237	0.3260	0.3238	0.4001	0.3996	0.1529	0.1529
25	33.33	32.80	160.77	160.44	0.0814	0.0834	0.2706	0.2688	0.4373	0.4371	0.2106	0.2108
26	33.33	33.33	163.24	163.43	0.0491	0.0504	0.2035	0.2022	0.4484	0.4484	0.2990	0.2990

4. DISCUSSION

To simulate the multicomponent distillation column, computer programs have been developed for four variations in Thiele-Geddes method. These program codes are given in Appendix-I. The standard example problems, which have been presented in Appendix-II, are used for simulation using the programs. The results of simulation studies are compared with results obtained using Hysys. The Results of the simulation using TGXBPTH and Hysys presented in Table 2-10, have been compared and the results of simulations obtained by using the remaining programs are presented in Appendix-III. Comparison between simulation results obtained from the computer programs using the example problems and those of Hysys are shown in Fig 4-54. It is observed that the compositions and temperature are obtained in present work for the example problems are in good agreement with those of Hysys.

4.1. INITIAL VALUE OF θ IN THE θ CONVERGENCE METHOD

With new temperatures estimates for the reboiler and for every plate within the column, new K values are determined for every component on every plate, and the entire cycle of calculations is repeated until convergence to the true solution is obtained. Convergence to the true solution will be indicated by a θ value of unity for that cycle and compositions and temperatures of the plates in the column being the same on successive cycles, within a prescribed value of error.

Careful study of the Newton iteration procedure and its graphical implications reveals that if the initial choice of θ is zero, the Newton iteration procedure will converge nicely, with the value of θ_i always increasing toward the correct value of θ that satisfies the criterion. Therefore, it is often recommended that the initial guess for θ be taken as zero. This will avoid any complications of encountering negative values of θ and in return the convergence problems with the Newton iteration procedure. On the other hand, as the convergence is approached in the Thiele-Geddes calculation, the value of θ for each cycle will get closer and closer to unity, and some computer time can usually be saved by initiating the Newton iteration procedure with a θ value of unity, rather than zero. If this is done, a safeguard must be employed to ensure a positive value of θ avoiding a negative value of θ_{i+1} in the iterative calculations. In all the simulations in the present work, convergence has been quite

Table - 11: Theta Values and Number of Iterations Taken by Each program for convergence

EXAMPLE	THETA				NUMBER OF ITERATIONS			
	TGXBP	TGXBPTH	TGXKBTH	TGCKBTTH	TGXBP	TGXBPTH	TGXKBTH	TGCKBTTH
Depropanizer-I	1.0047	1.0001	1.0002	1.0001	20.	7	9	9
Paraffin separation	1.0000	0.999992	0.999998	1.000	11	10	11	11
Depropanizer-II	0.9936	1.0002	0.9999	0.9999	20	11	9	9
Ethane splitter	1.0006	0.9999	1.0001	1.0000	20	8	9	10
Xylene fractionation	0.9894	0.9998	0.9999	0.9999	20	10	11	11
Ethyl benzene- styrene separation	0.9999	0.9999	1.00001	1.0000	20	11	14	14
Separation of toluene-ethyl benzene	0.9999	1.0000	1.0000	1.0000	20	13	13	13
Biphenyl separation	1.0005	1.0002	0.9996	0.9995	20	6	8	8
Phenol- cresol separation	1.0003	1.0000	1.0000	1.0000	20	7	8	8

satisfactory with the initial value of θ equal to zero. However, the initial guess values for top and bottom temperatures influenced greatly leading to convergence problems.

4.2 NUMBER OF ITERATIONS FOR CONVERGENCE

The numbers of iterations taken by each program to attain convergence for simulations are presented in Table 11. As seen from Table 11, the program TGXBPTH has taken less number of iterations compared to those taken by the other programs. In the programs, the convergence criterion has been set for a maximum of 20 iterations. Initial guess values have a profound effect on the convergence for all the example problems when this program is used for simulation. The last two programs, TGXKBTH and TGCKBTTH, have taken same number of iterations for convergence. This means the Thomas algorithm has no effect on iterative calculations for the chosen example problems.

4.3 SUMMARY OF OBSERVATIONS ON SIMULATIONS WITH EXAMPLES

EXAMPLE 01: DEPROPANIZER –I

The average deviations in temperature and compositions profiles for depropanizer-I in rectifying and stripping sections are presented in Table-12.

As shown in Fig-4 the temperature profile for rectifying section has been predicted in both the simulations of Hysys and present work. For the stripping section the variation is in the range of 4.9 °C. There exits very good agreement for the liquid compositions profile of ethane in both the cases of simulations. With respect to Propane (LK) slightly higher liquid compositions profiles are predicted for rectifying section by the present simulation program compared to the Hysys simulation. Whereas the trend is reversed in stripping section, in contrast marginal higher liquid composition profile for I-butane has predicated by the Hysys program for rectifying section and the same trend is reversed in the stripping section. A little variation in the profile of n-pentane is observed below the feed plate.

Table 12: Average deviation in rectifying and stripping sections for depropanizer-I

Depro-panizer-I	T °C		ethane		propane		i-butane		n-butane		n-pentane	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	1.73	4.90	0.000	0.000	0.016	0.024	0.006	0.014	0.008	0.015	0.001	0.006

R.S = Rectifying section; **S.S** = Stripping section

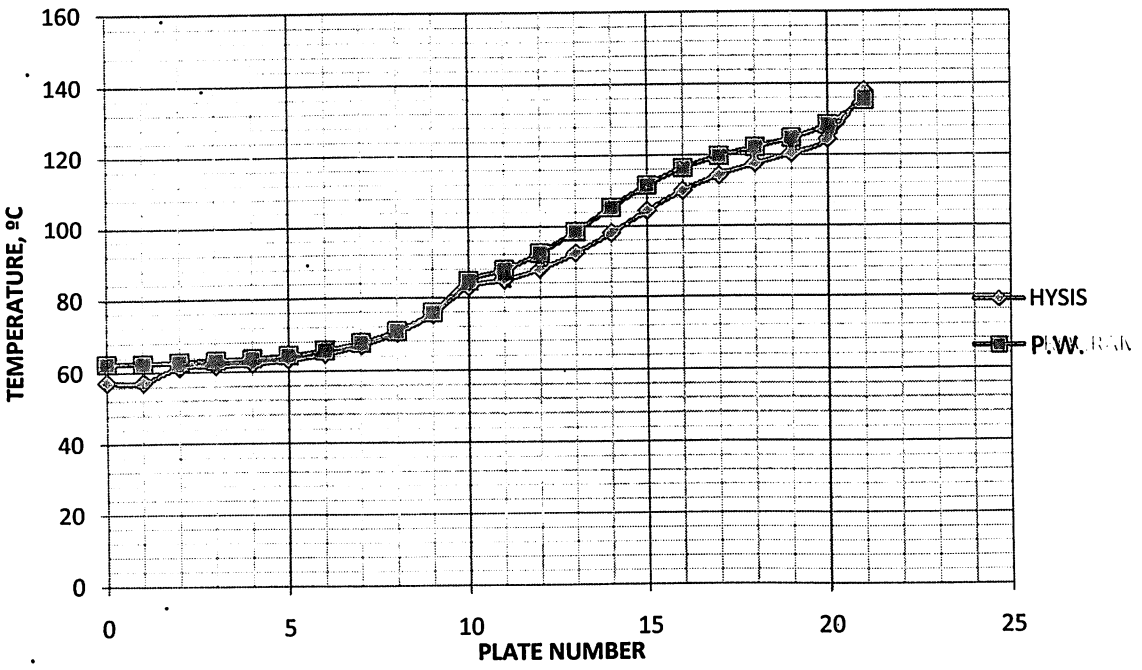

Figure 4: Temperature profile for the Depropanizer-I

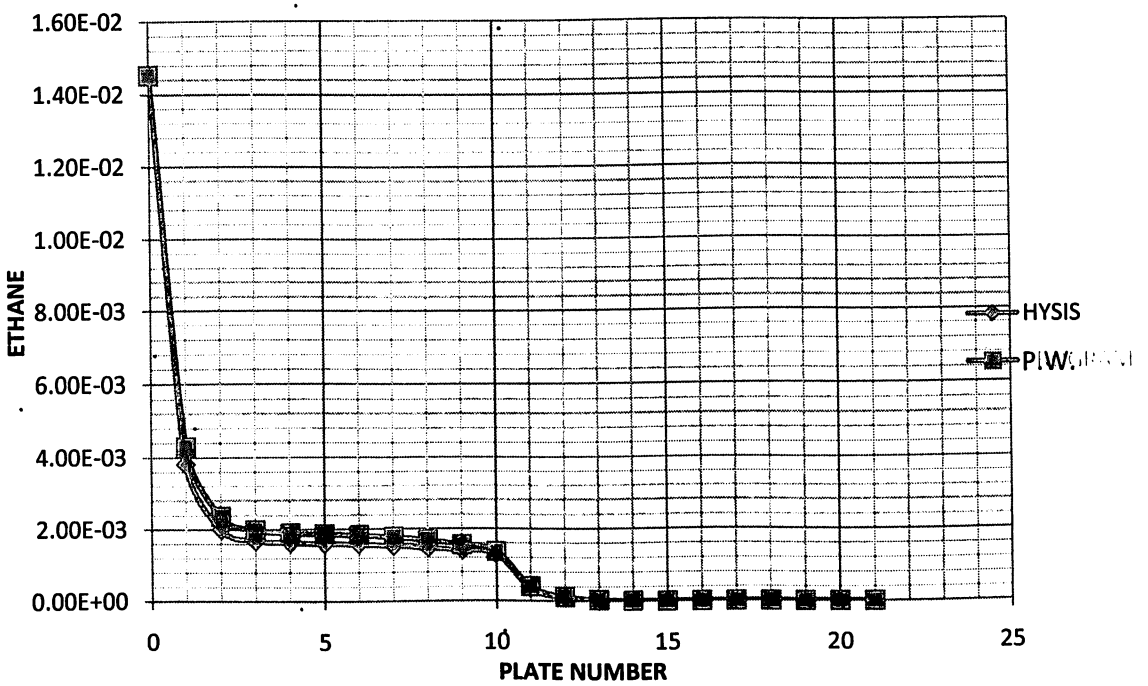

Figure 5: Ethane liquid composition profile for the Depropanizer-I

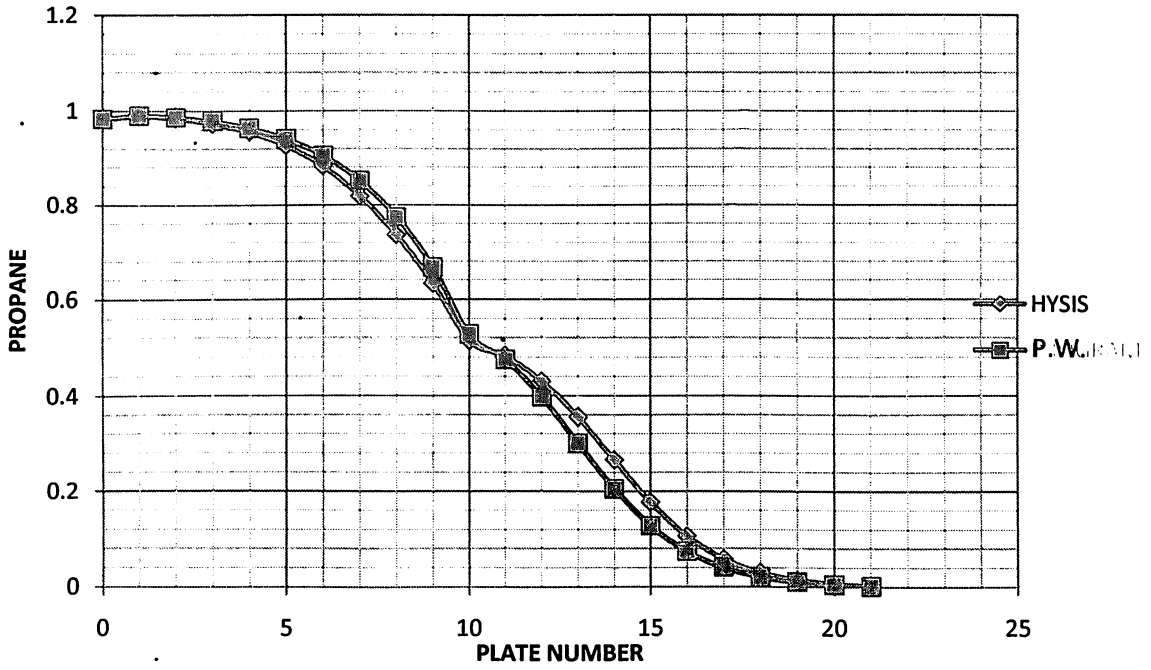

Figure 6: Propane liquid composition profile for the Depropanizer-I

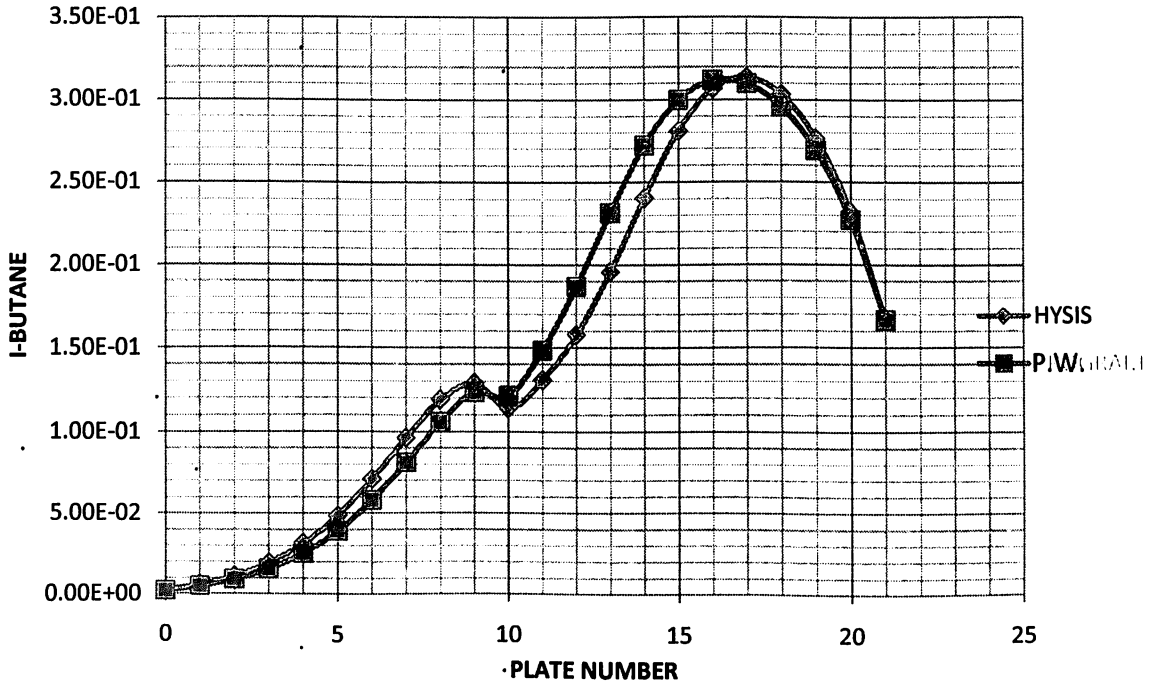

Figure 7: I-butane liquid composition profile for the Depropanizer-I

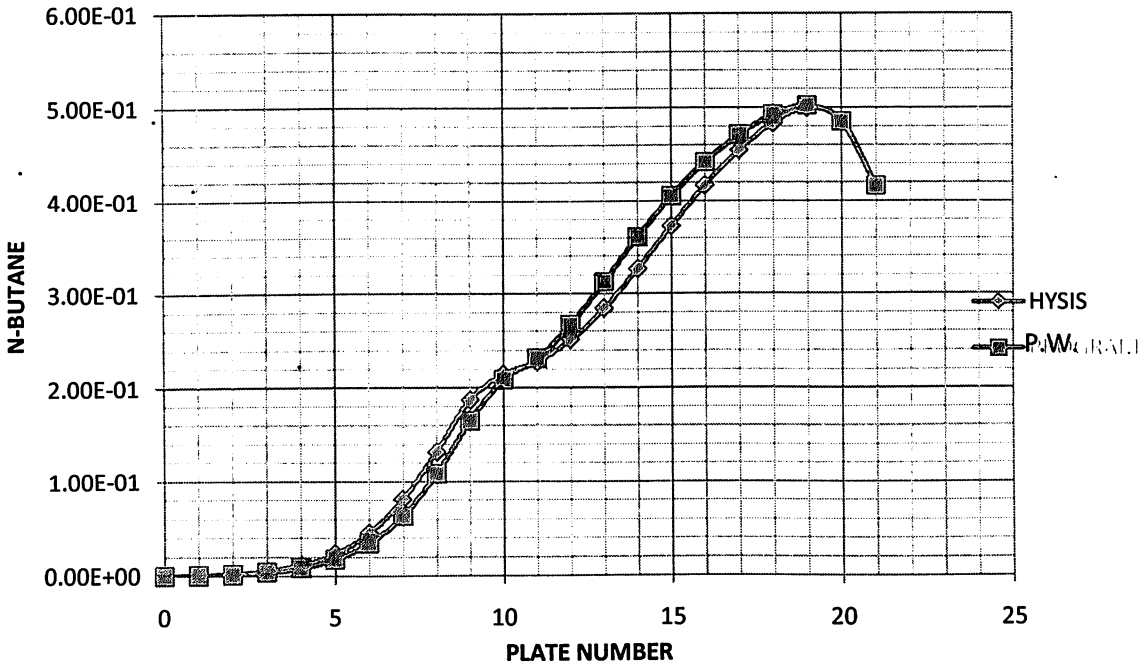

Figure 8: N-butane liquid composition profile for the Depropanizer-I

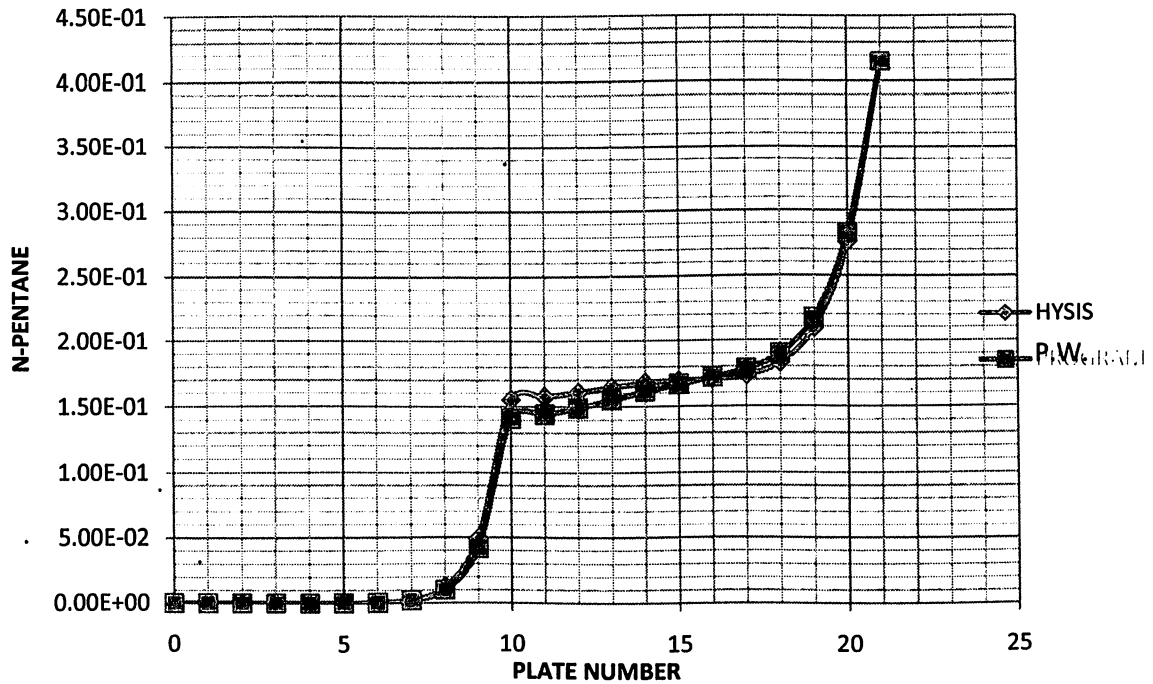

Figure 9: N-pentane liquid composition profile for the Depropanizer-I

EXAMPLE 02: PARAFFIN SEPARATION

This is an example taken from the fractionation of linear alkyl benzene. The average deviations in temperature and compositions profiles for paraffin separation in rectifying and stripping sections are presented in Table-13. Both the simulations have resulted almost identical temperature profile as shown in Fig-10. Expect for slight variations in rectifying section, the prediction profile of nonane in the stripping section, as is observed from the Fig-11 by both the cases of simulation is in excellent agreement. As shown in Fig-12-15, slightly high composition profiles are found for n-decane, undecane and n-tridecane in the rectifying section and highly compatible profiles in the stripping section.

Table 13: Average deviation in rectifying and stripping section for paraffin separation

Paraffin separation	T °C		nonane		n-decane		undecane		n-dodacane		n-tridecane		n-tetra decane	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	2.47	0.16	0.004	0.001	0.035	0.002	0.030	0.001	0.055	0.001	0.011	0.000	0.000	0.000

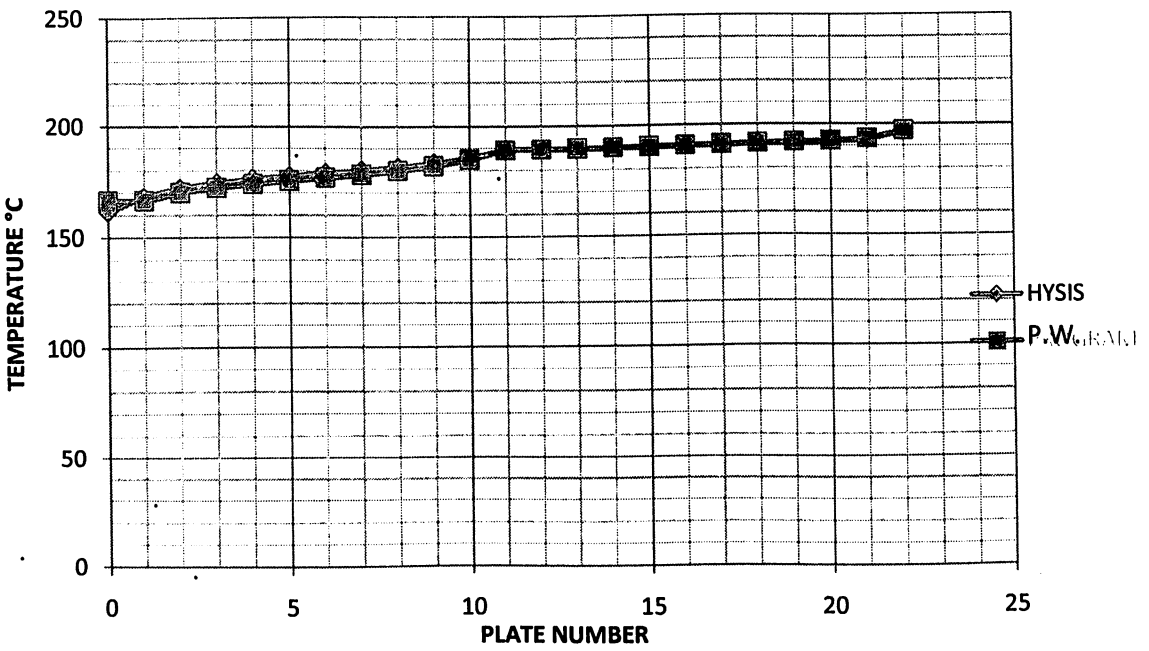

Figure 10: Temperature profile for the Paraffin separation

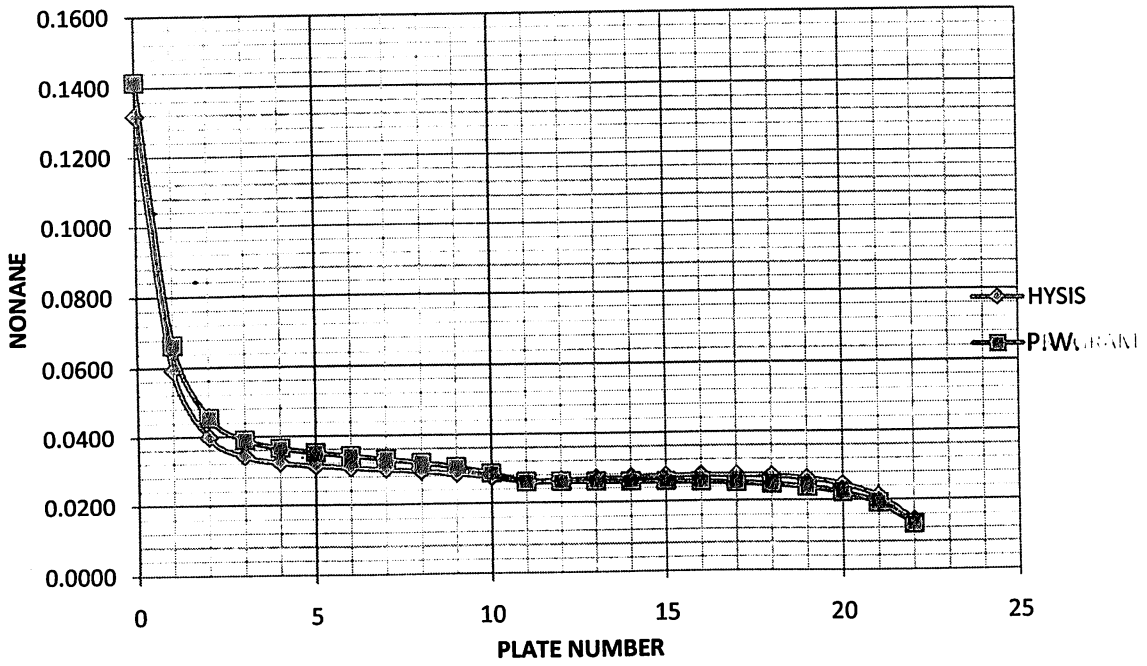

Figure 11: Nonane liquid composition profile for the Paraffin separation

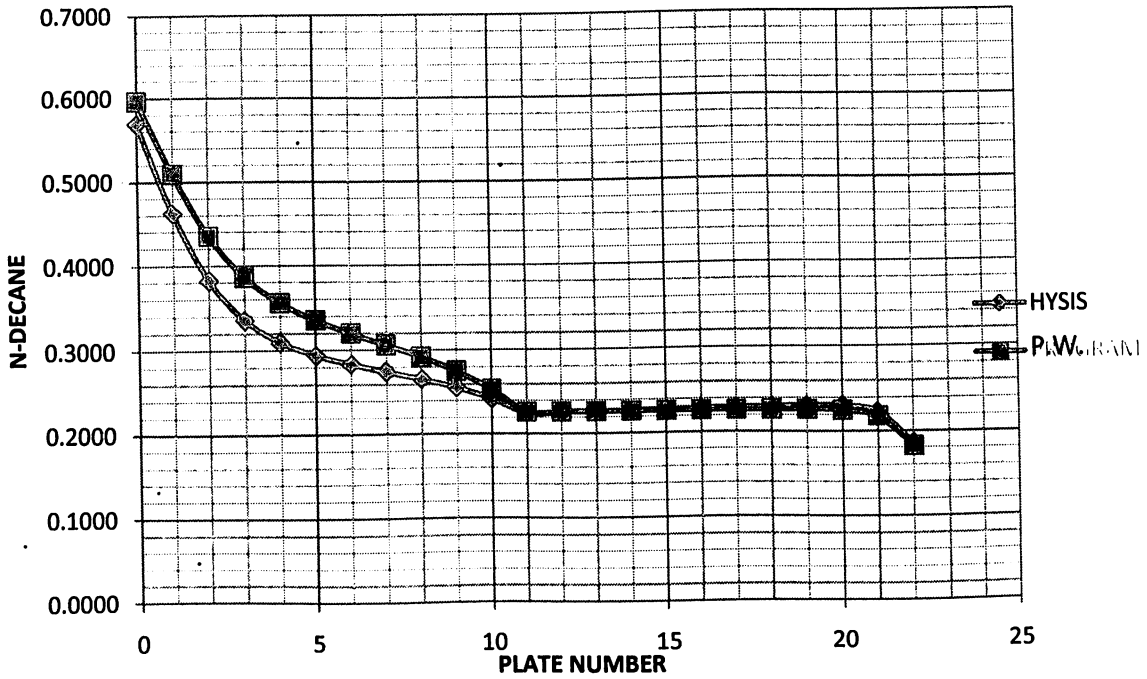

Figure 12: N-decane liquid composition profile for the Paraffin separation

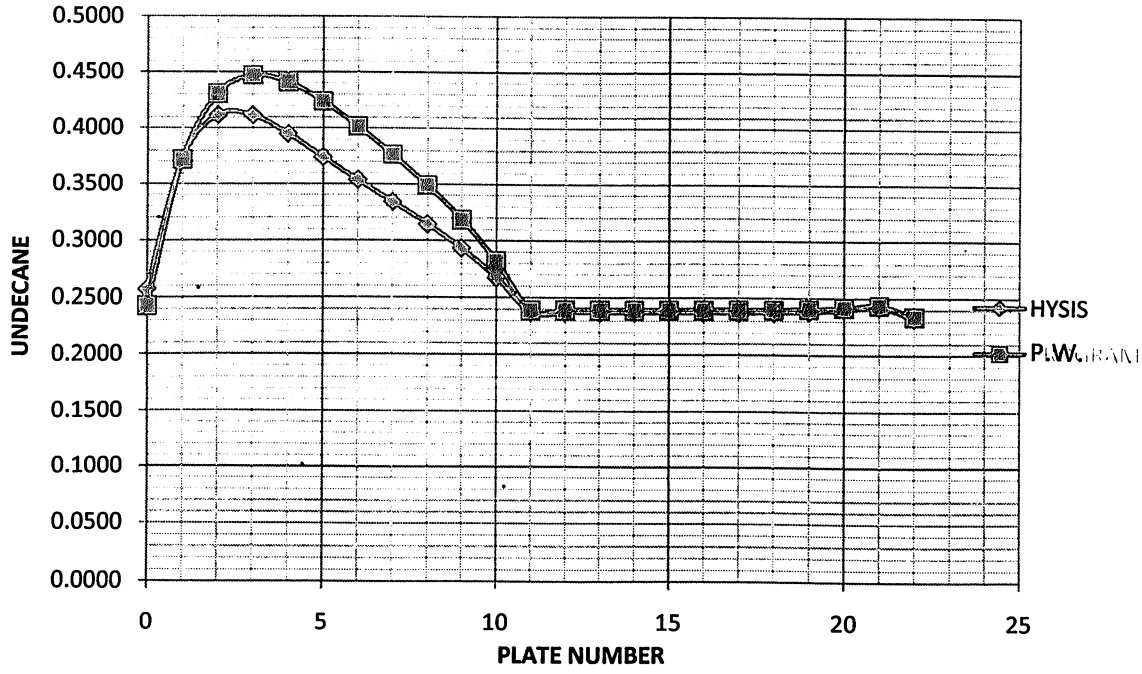

Figure 13: Undecane liquid composition profile for the Paraffin separation

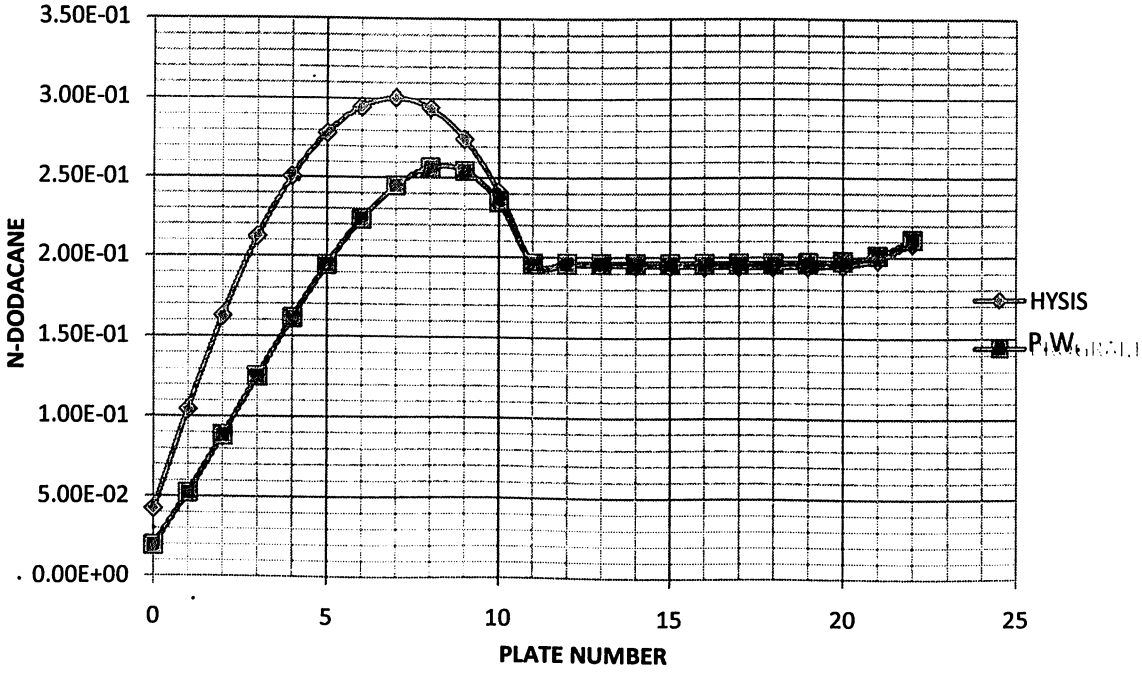

Figure 14: N-decane liquid composition profile for the Paraffin separation

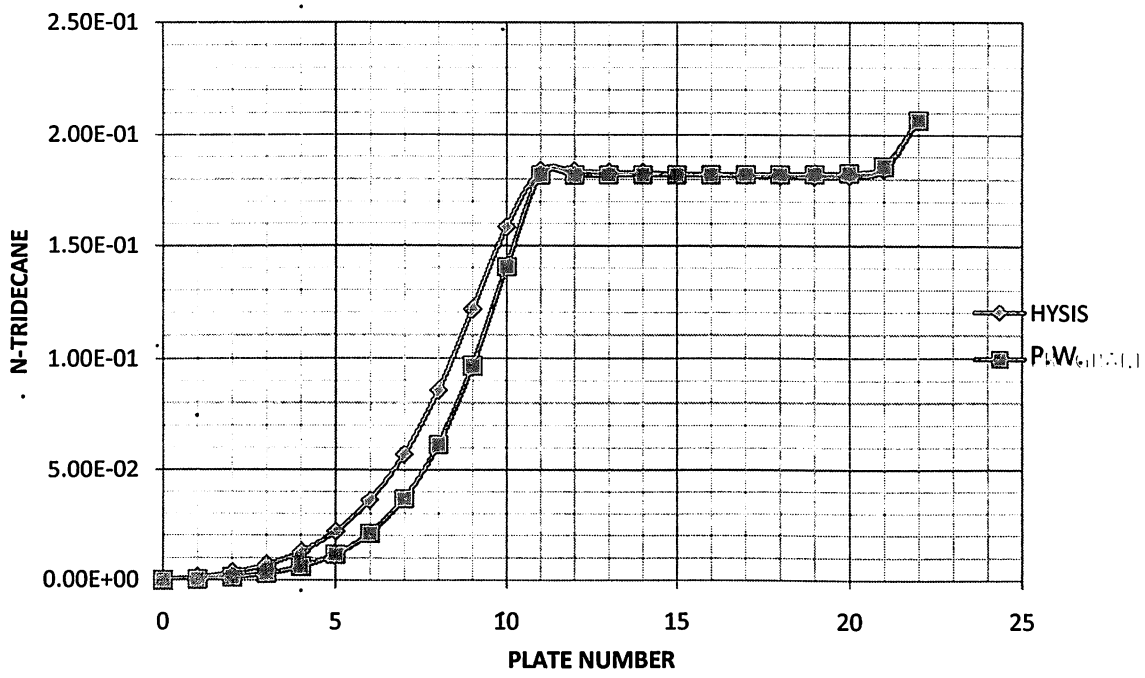

Figure 15: N-tridecane liquid composition profile for the Paraffin separation

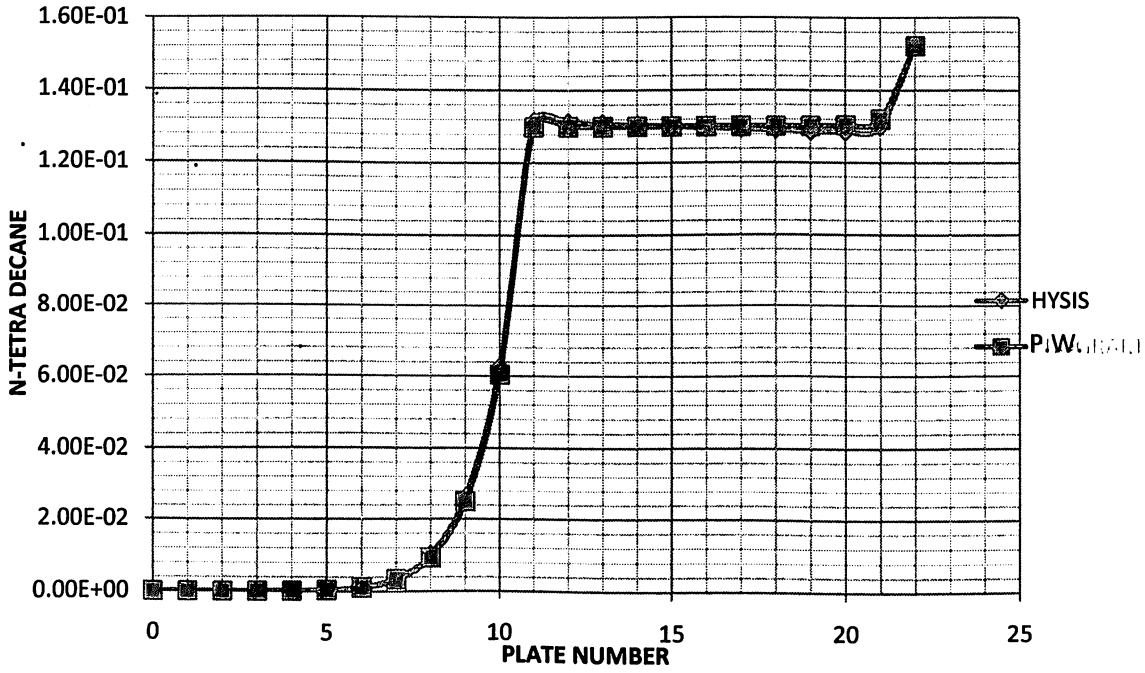

Figure 16: N-tetradecane liquid composition profile for the Paraffin separation

EXAMPLE 03: DEPROPANIZER-II

The average deviations in temperature and compositions profiles for depropanizer-II in rectifying and stripping sections are presented in Table-14. As shown in Fig-16, the temperature profile for rectifying section has been predicted identical in both the simulations of Hysys and present work. For the stripping section, the average deviation is in the range of 9 °C. There exits very good agreement for the liquid compositions profile of methane in both the cases of simulations as shown in Fig-17. As shown in Fig-18-23, low composition profiles are found for ethane in the rectifying section and highly compatible profiles in the stripping section. Whereas this trend is reversed for the propane, n-butane, n-pentane and n-hexane.

Table 14: Average deviation in rectifying and stripping section for depropanizer-II

Depropanizer-II	T °C		methane		ethane		propane		n-butane		n-pentane		n-hexane	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	0.80	9.63	0.005	0.000	0.006	0.000	0.019	0.087	0.006	0.061	0.000	0.026	0.000	0.023

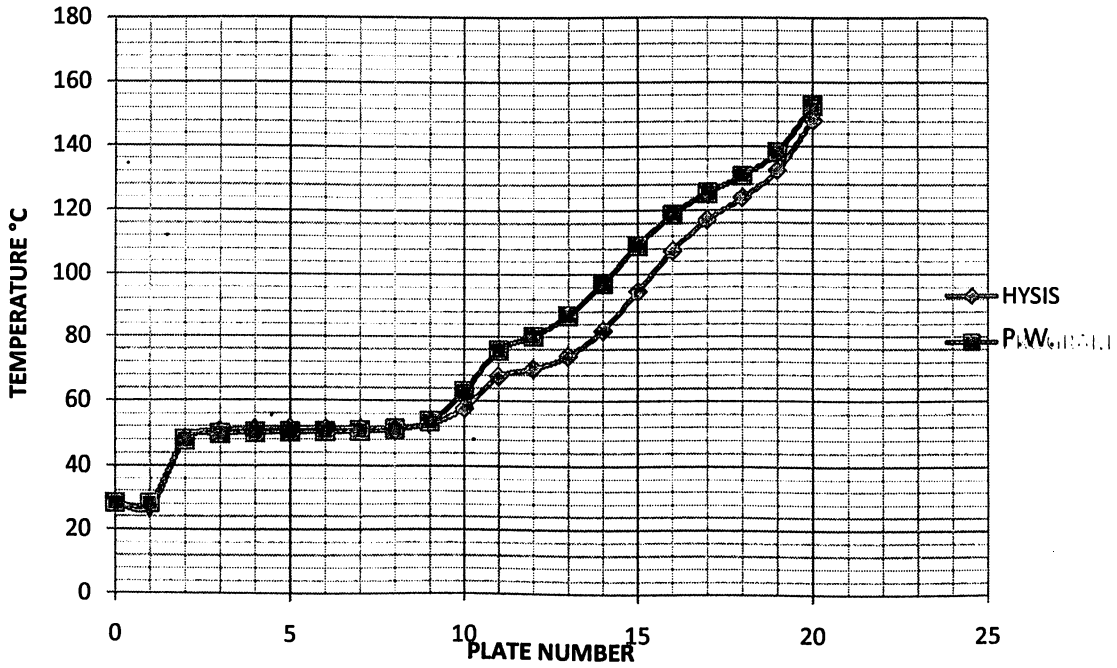

Figure 17: Temperature profile for the Depropanizer-II

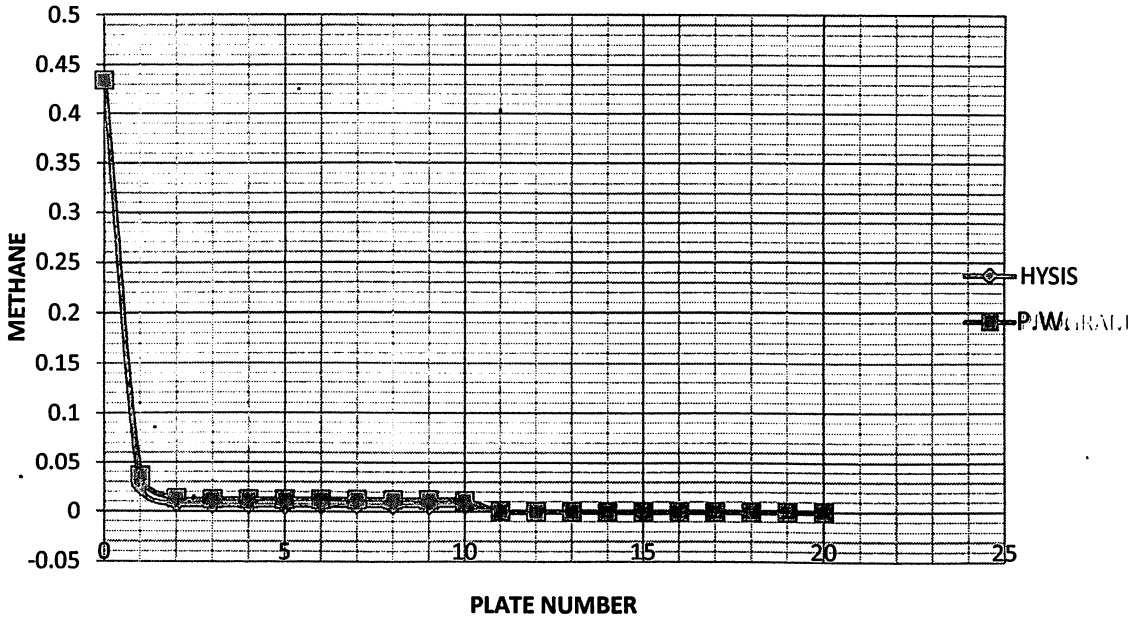

Figure 18: Methane liquid composition profile for the Depropanizer-II

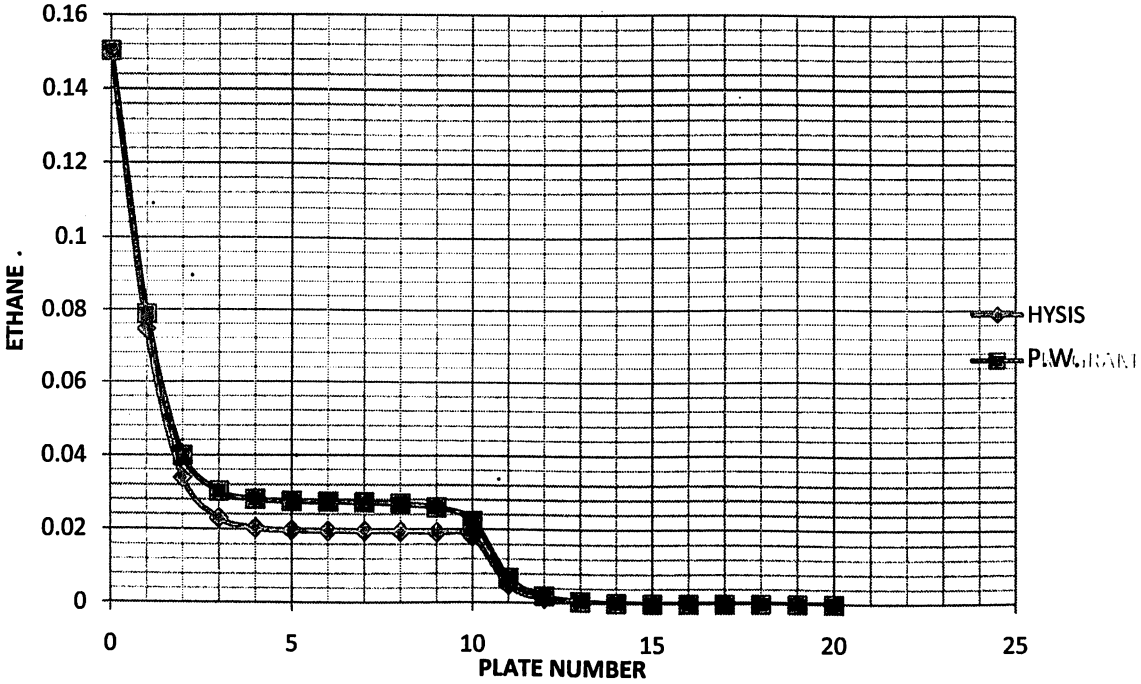

Figure 19: Ethane liquid composition profile for the Depropanizer-II

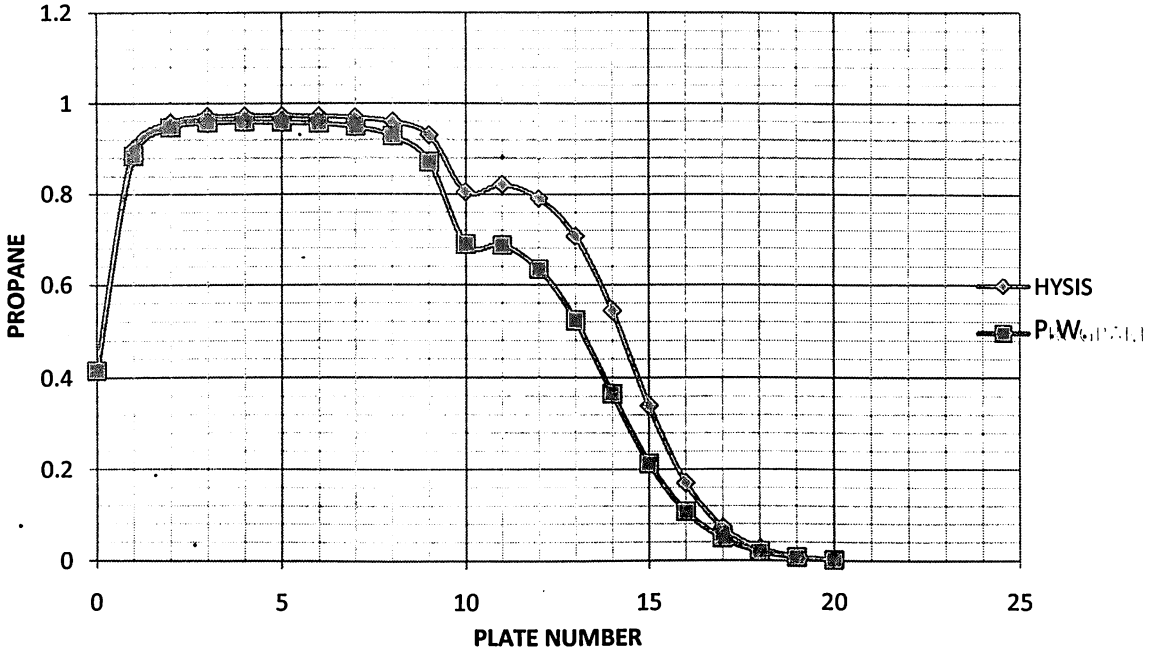

Figure 20: Propane liquid composition profile for the Depropanizer-II

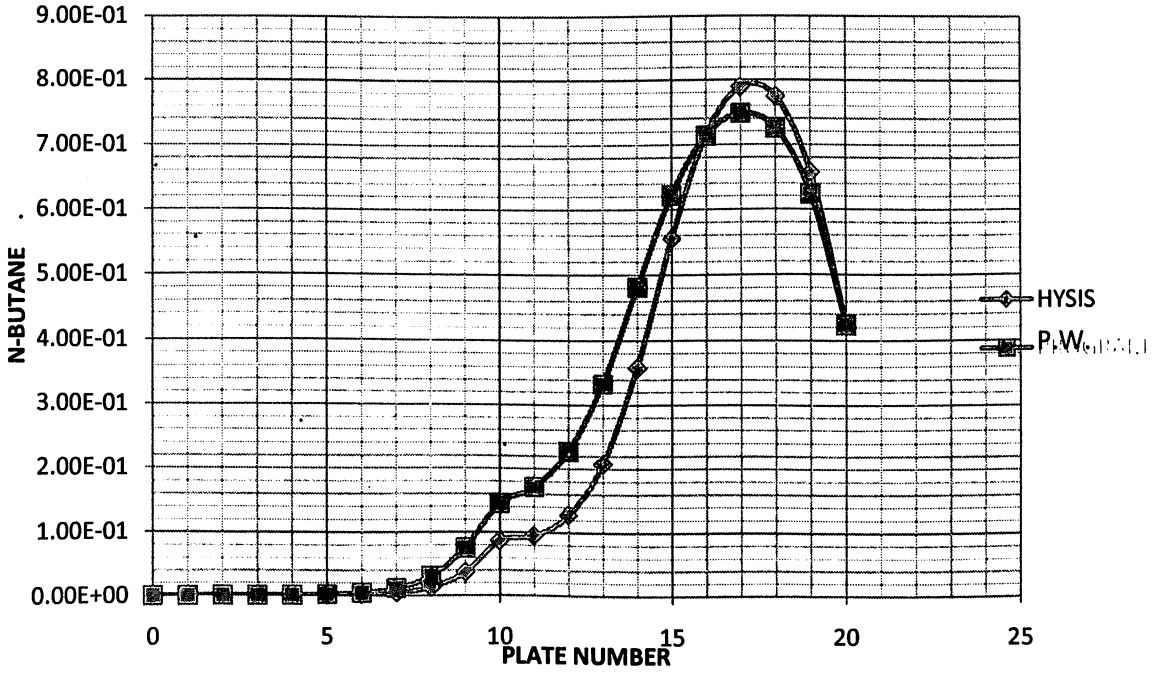

Figure 21: N-butane liquid composition profile for the Depropanizer-II

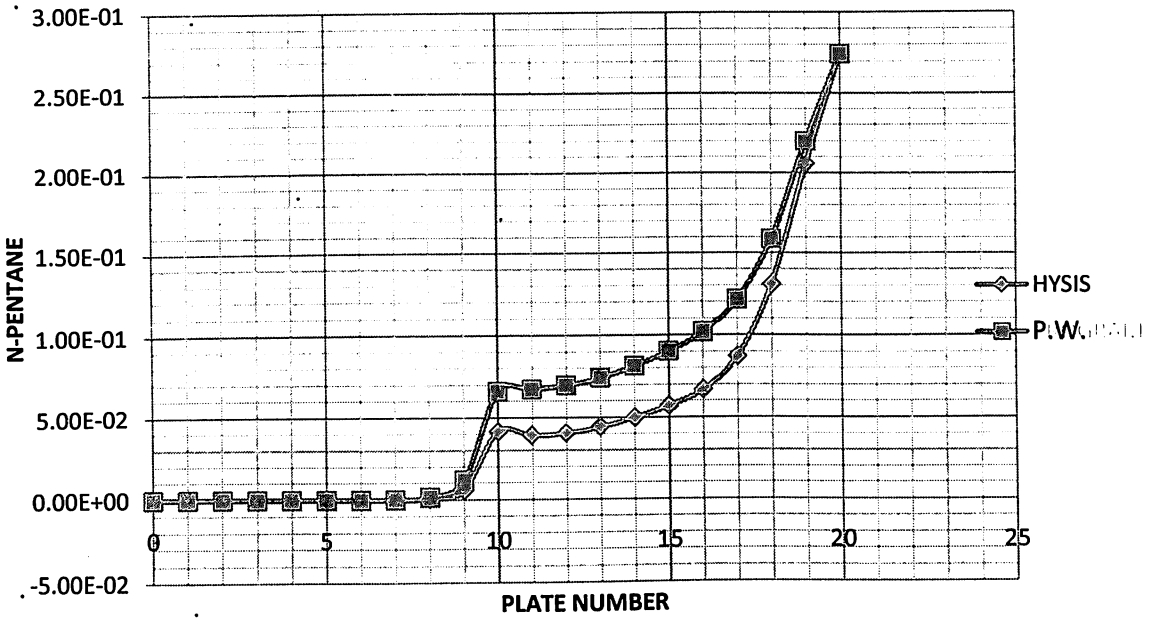

Figure 22: N-pentane liquid composition profile for the Depropanizer-II

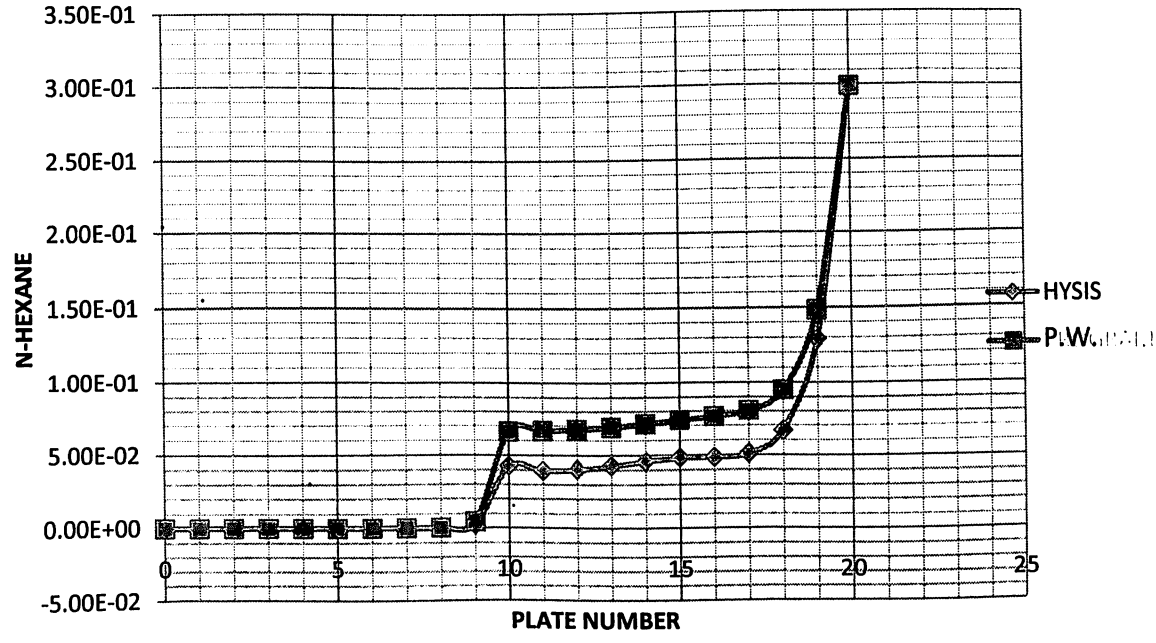

Figure 23: N-hexane liquid composition profile for the Depropanizer-II

EXAMPLE 04: ETHANE-SPLITTER

This example represents a mixture from cracking operations in a refinery excluding ethylene. The column operates at about 27 atm compared to the depropanizer examples which are set at 18 atm.

The average deviations in temperature and compositions profiles for ethane splitter in rectifying and stripping sections are presented in Table-15. As shown in Fig-25 the temperature profile for rectifying section has been predicted almost identical in both the simulations of Hysys and present work. For the stripping section the variation is in the range of 7.33 °C. Expect for slight variations in stripping section, the prediction of composition profile of all components in the rectifying section, as is observed from the Fig-25-30 by both the cases of simulation is in excellent agreement

Table 15: Average deviation in rectifying and stripping section for ethane splitter

Ethane splitter	T °C		methane		ethane		propylene		propane		i-butane		n-butane	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	1.85	7.33	0.002	0.000	0.015	0.047	0.006	0.018	0.005	0.019	0.000	0.004	0.000	0.006

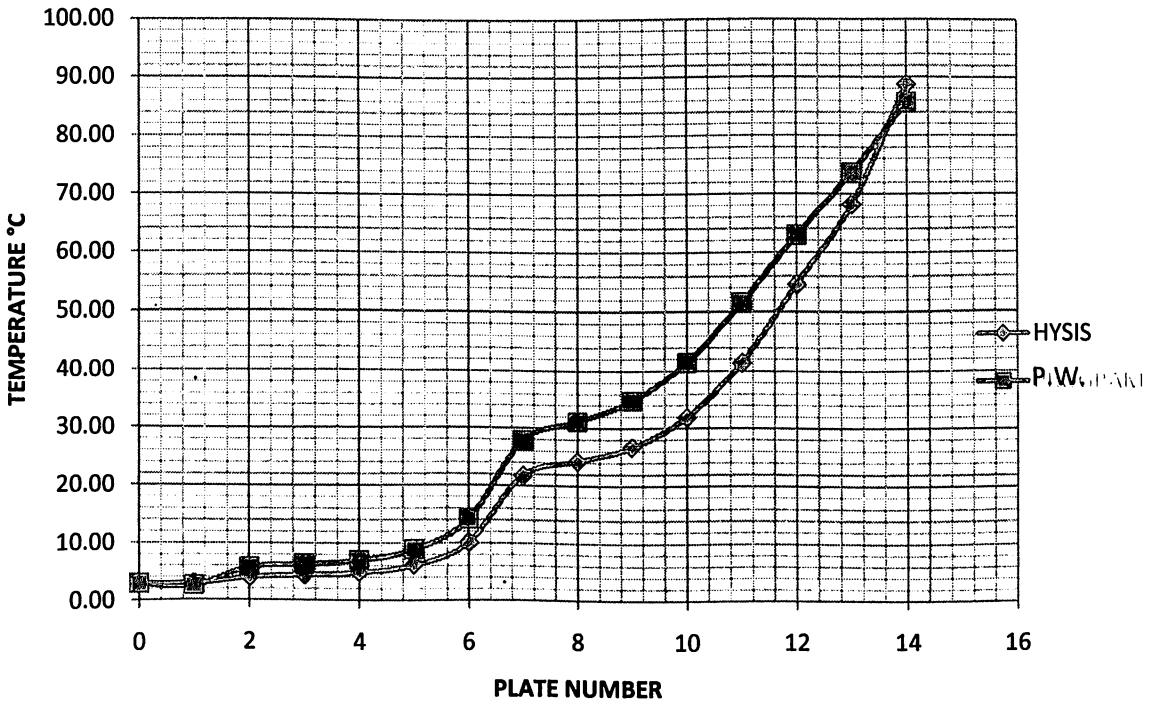

Figure 24: Temperature profile for the Ethane splitter

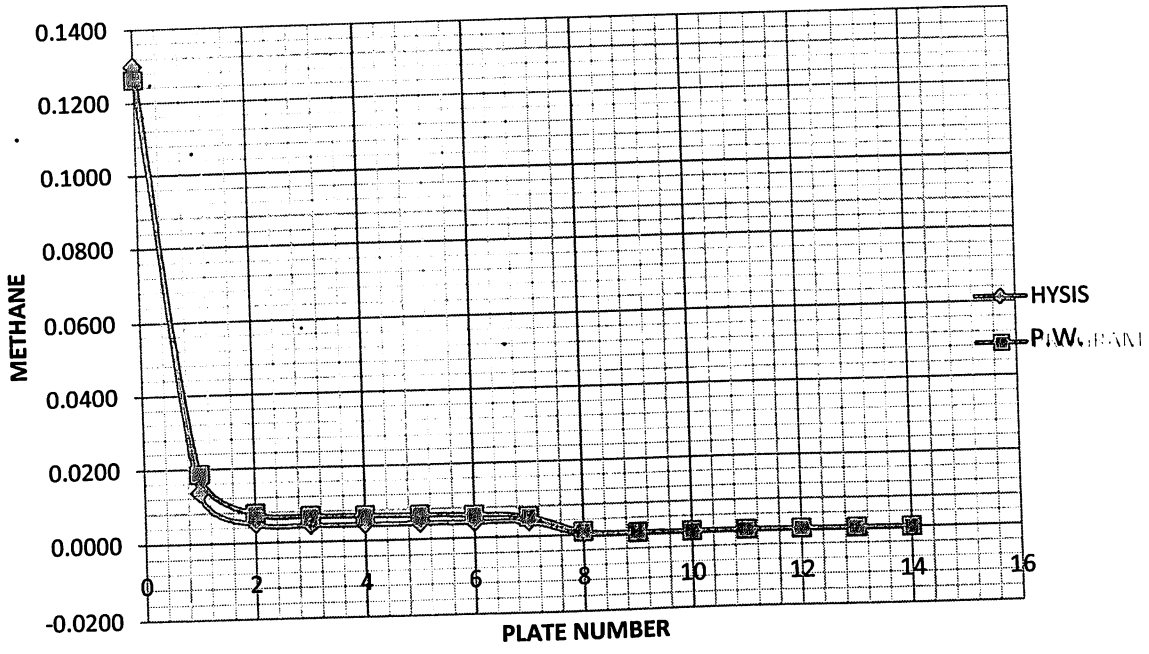

Figure 25: Methane liquid composition profile for the Ethane splitter

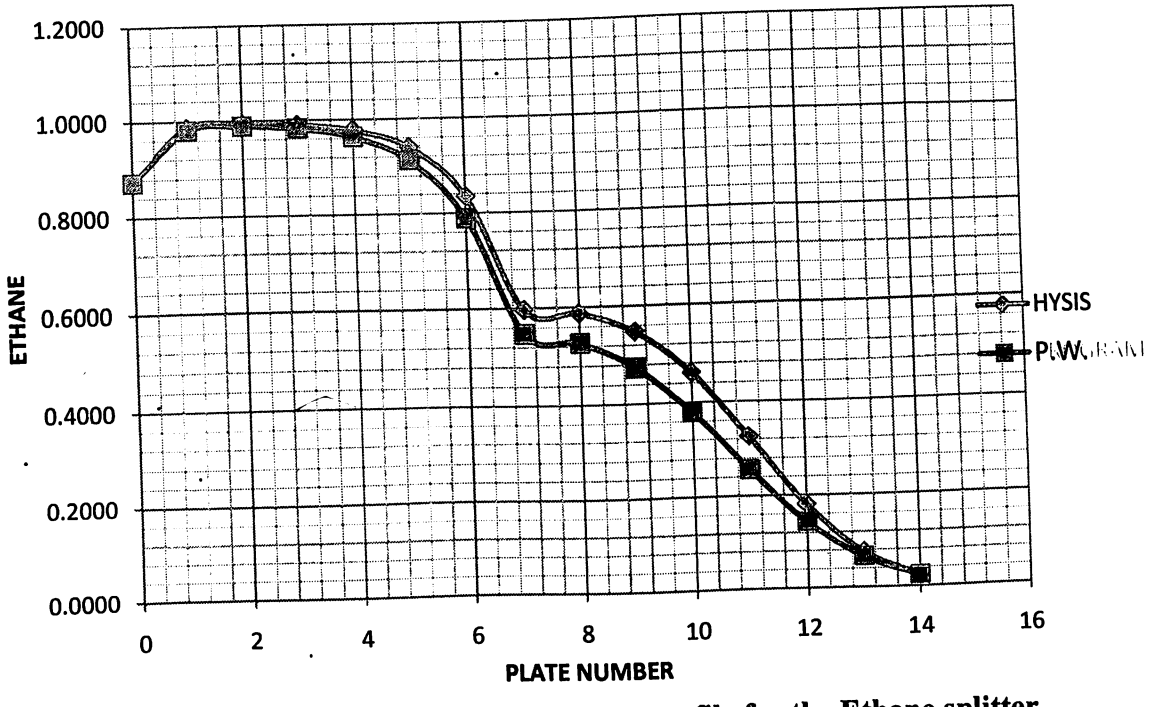

Figure 26: Ethane liquid composition profile for the Ethane splitter

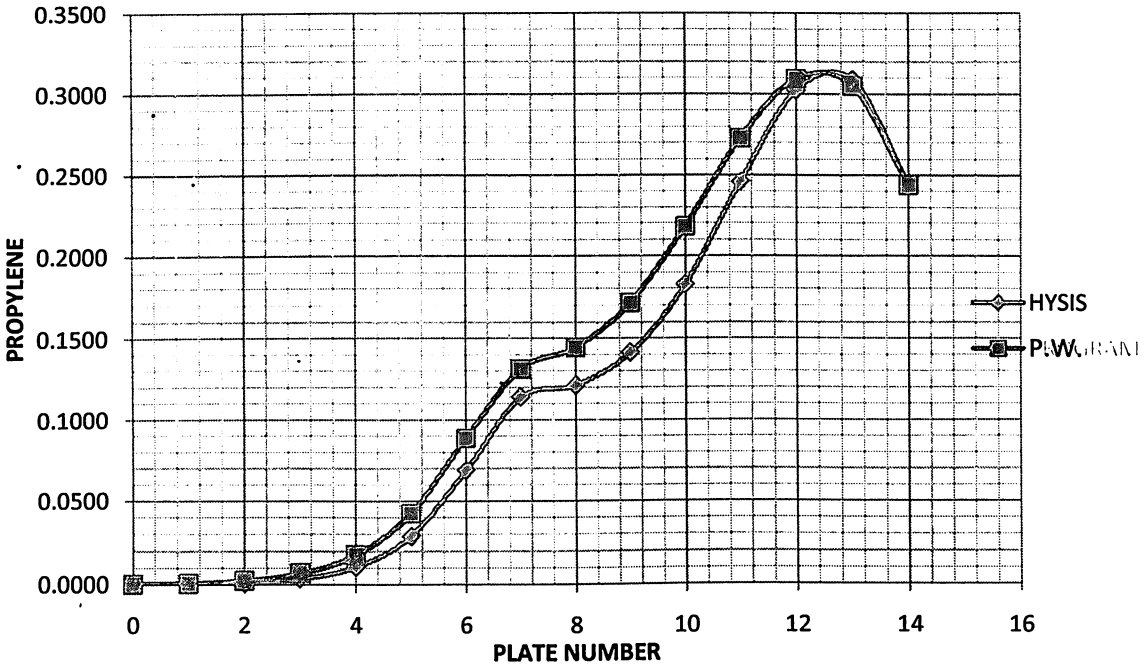

Figure 27: Propylene liquid composition profile for the Ethane splitter

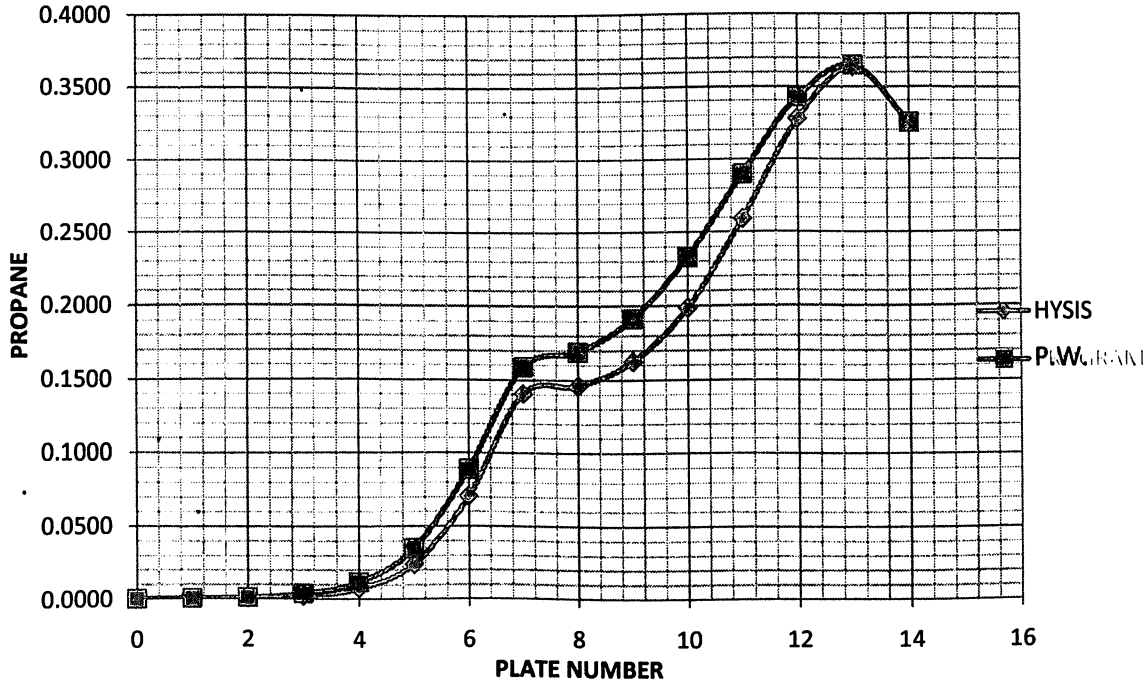

Figure 28: Propane liquid composition profile for the Ethane splitter

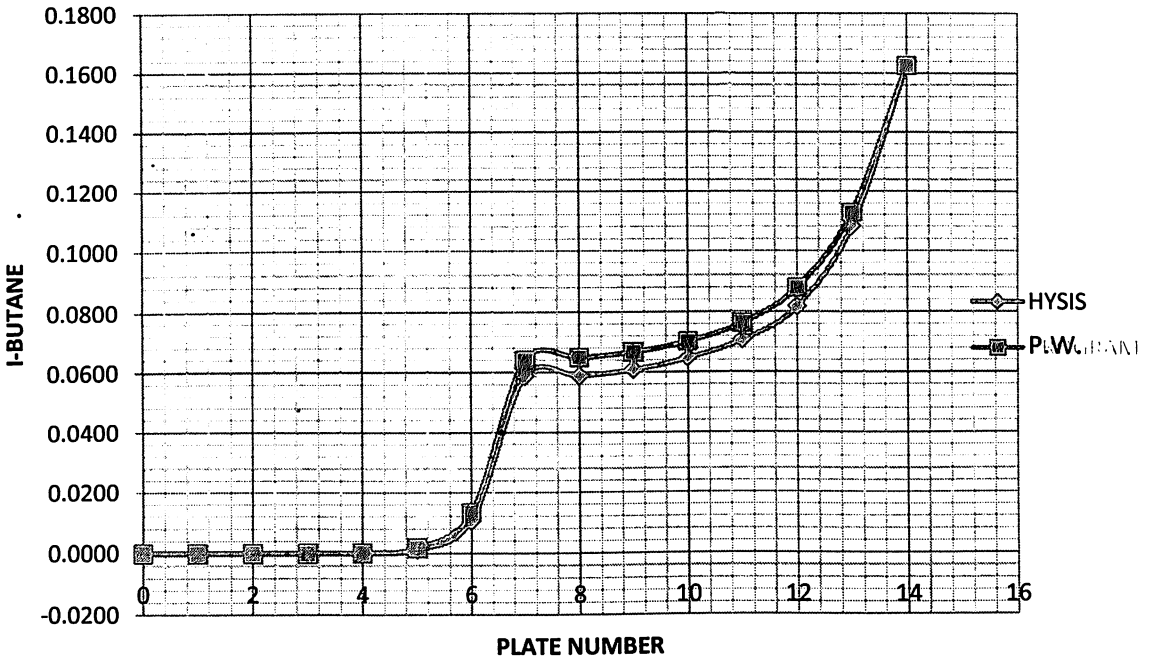

Figure 29: I-butane liquid composition profile for the Ethane splitter

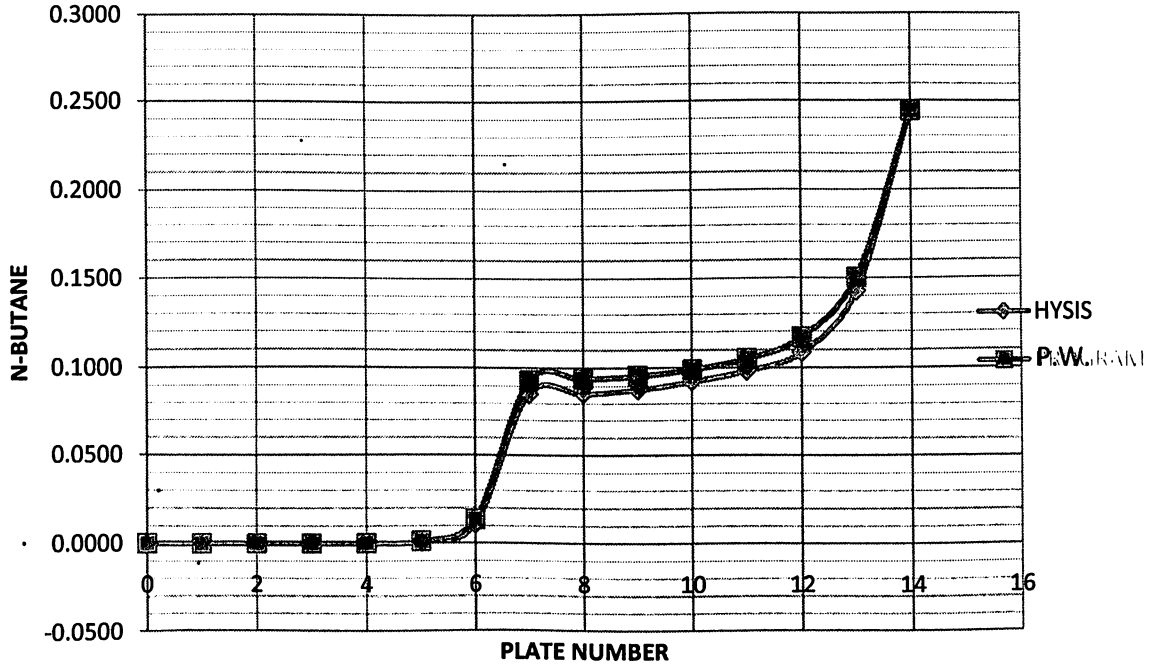

Figure 30: N-butane liquid composition profile for the Ethane splitter

EXAMPLE 05: FRACTIONATION-OF-XYLENES

The xylene separation is an example for a very close boiling component mixture and super fractionation. In industry, the distillation columns are operated at 3 atm , 8 atm and 12 atm because of heat integration though the relative volatility is very close to one. At hight pressure, the number of plates are usually around 300. In this work, the column pressure is set at 1 atm with 100 plates to get similar product distribution.

The average deviations in temperature and compositions profiles for xylene fractionation in rectifying and stripping sections are presented in Table-16. Both the simulations have resulted almost identical temperature profile as shown in Fig-31. As is observed from the Fig-32-35, there exits very good agreement for the liquid compositions profiles of all components in both the cases of simulations.

Table 16: Average deviation in rectifying and stripping section for xylene fractionation

Xylene fractionation	T °C		ethyl benzene		p-xylene		m-xylene		o-xylene	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	0.07	0.20	0.000	0.000	0.004	0.003	0.007	0.005	0.004	0.002

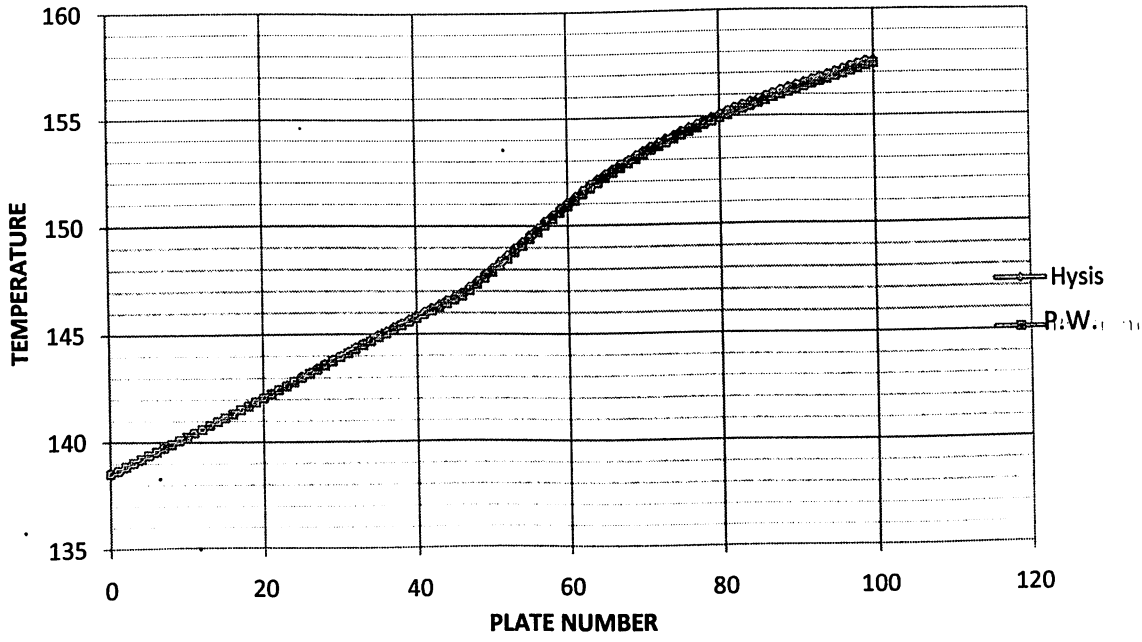

Figure 31: Temperature profile for the fractionation of Xylenes

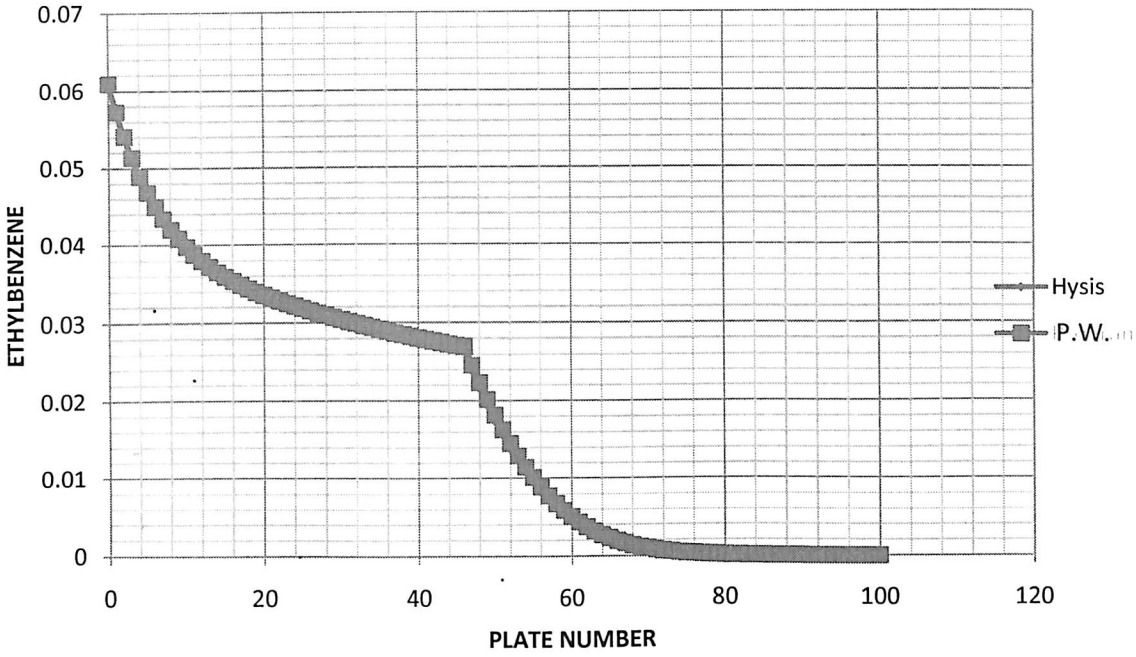

Figure 32: Ethylbenzene liquid composition profile for the fractionation of Xylenes

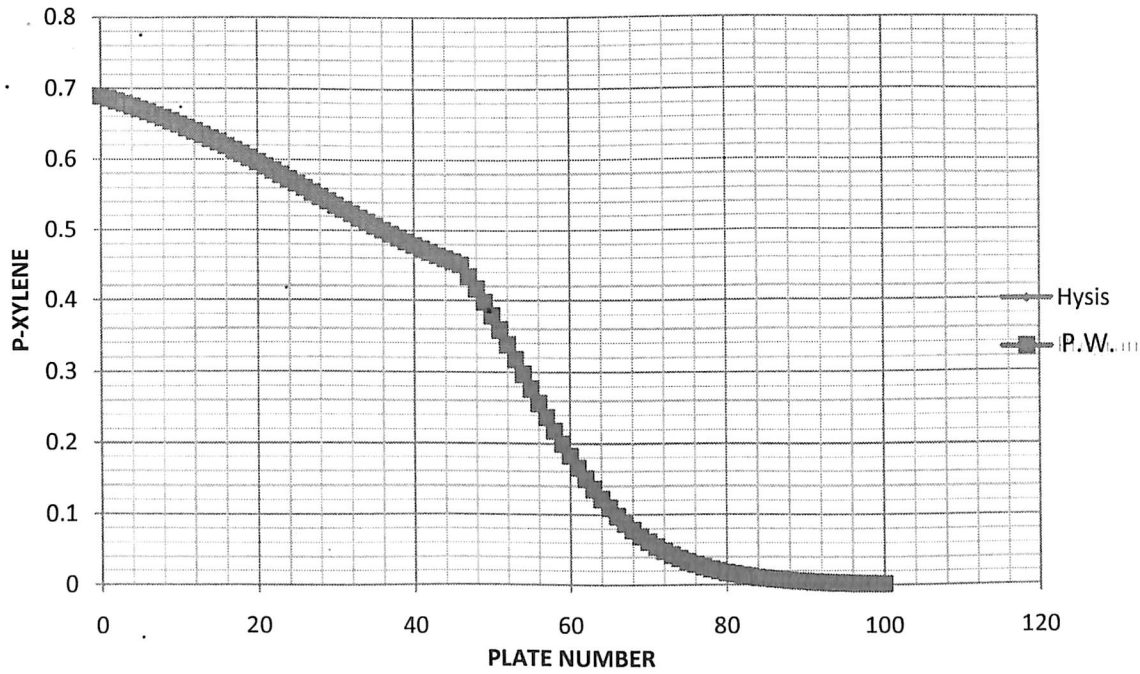

Figure 33: P-xylene liquid composition profile for the fractionation of Xylenes

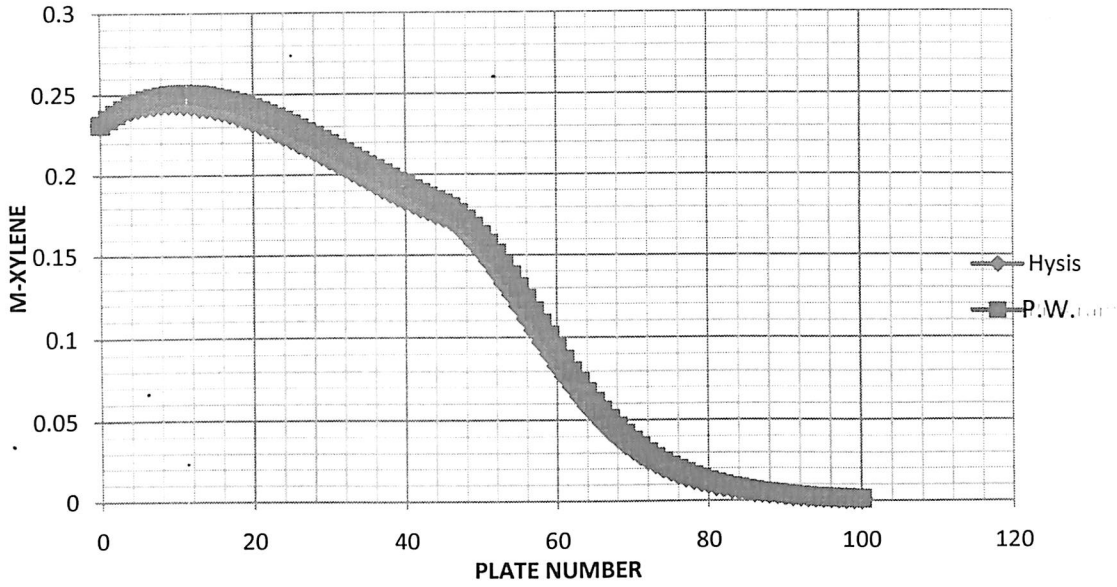

Figure 34: M-xylene liquid composition profile for the fractionation of Xylenes

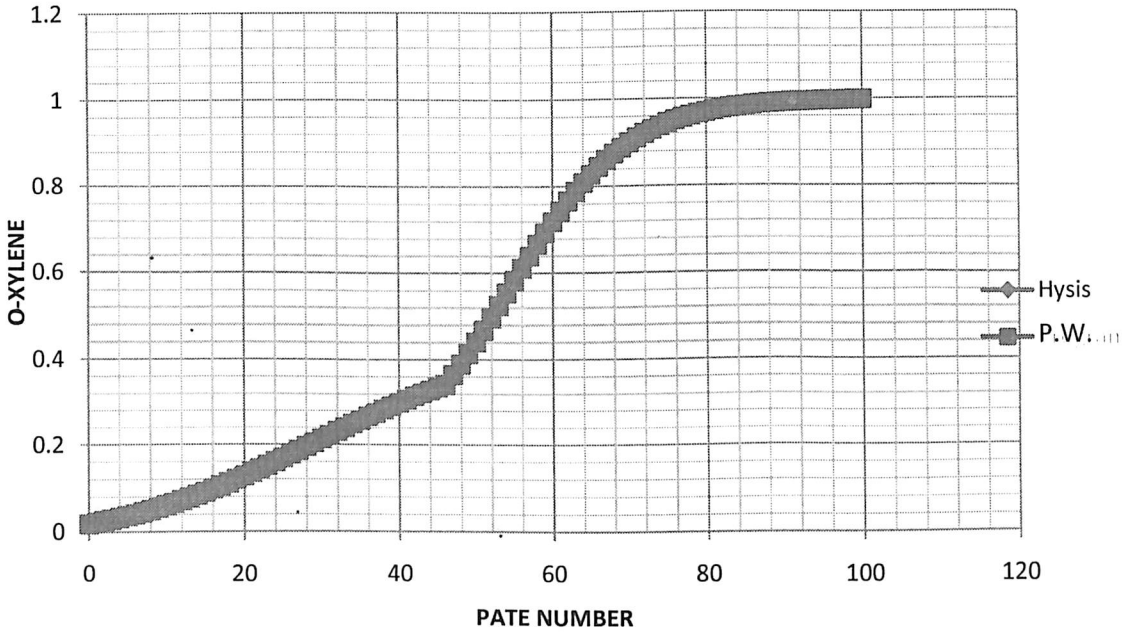

Figure 35: O-xylene liquid composition profile for the fractionation of Xylenes

EXAMPLE 06: SEPARATION OF ETHYLBENZENE-STYRENE

This mixture is a standard example to evaluate column internals. The separation also a good example for super fractionation carried out at very low pressure (vacuum).

The average deviations in temperature and compositions profiles for ethylbenzene-styrene separation in rectifying and stripping sections are presented in Table-17. Both the simulations have resulted almost identical temperature profile as shown in Fig-36.As is observed from the Fig-37-40 by There exits very good agreement for the liquid compositions profiles of all components in both the cases of simulations, expect for cumene. As shown in Fig-40, the composition profile, predicted in the present work, is found for cumene in the rectifying and stripping sections slightly higher than the Hysys simulation results.

Table 17: Average deviation in rectifying and stripping section for ethylbenzene-styrene separation

Ethyl benzene-styrene separation	T °C		toluene		ethyl benzene		styrene		cuemen	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	1.08	0.83	0.000	0.000	0.003	0.006	0.003	0.006	0.000	0.000

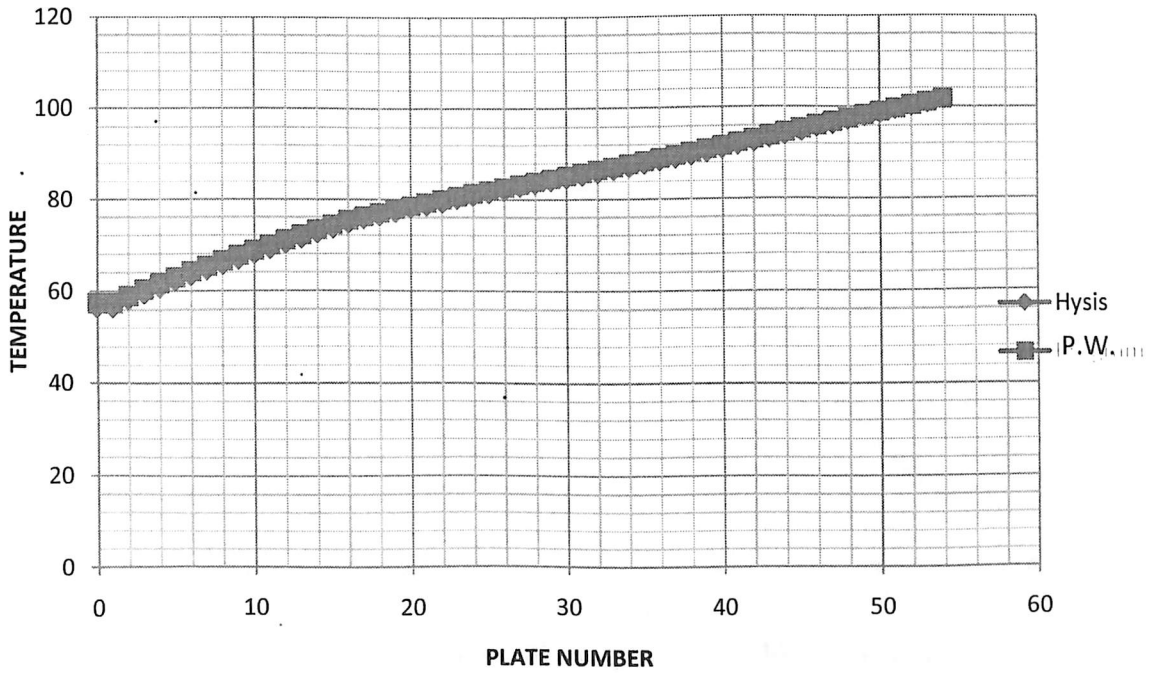

Figure 36: Temperature profile for the separation of EB - Styrene

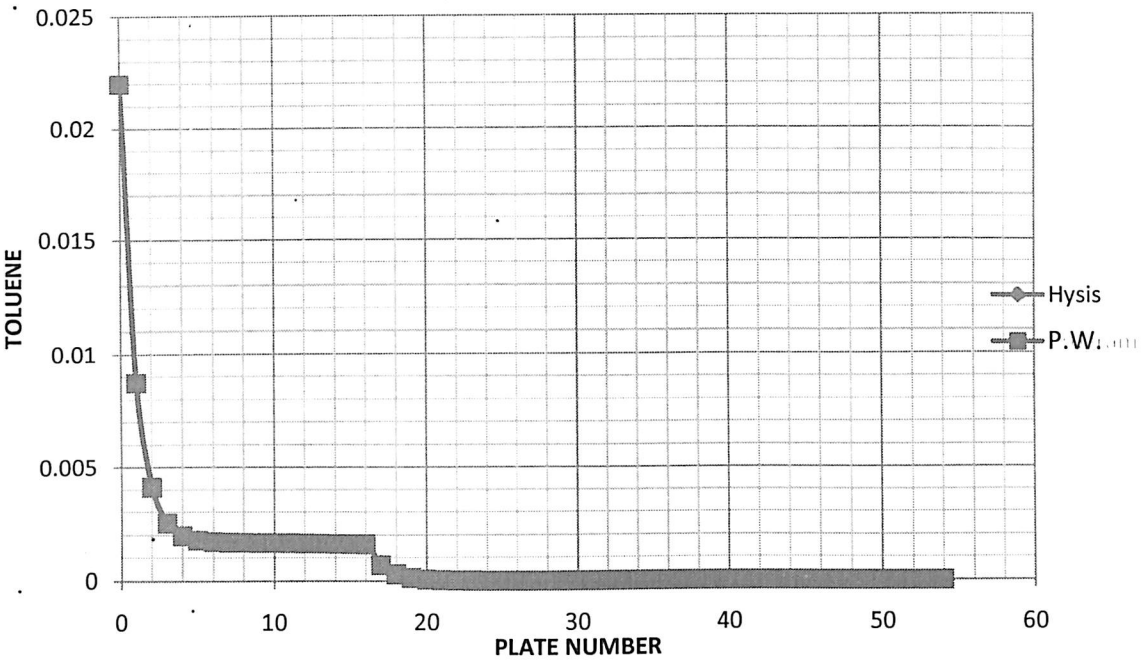

Figure 37: Toluene liquid composition profile for the separation of EB – Styrene

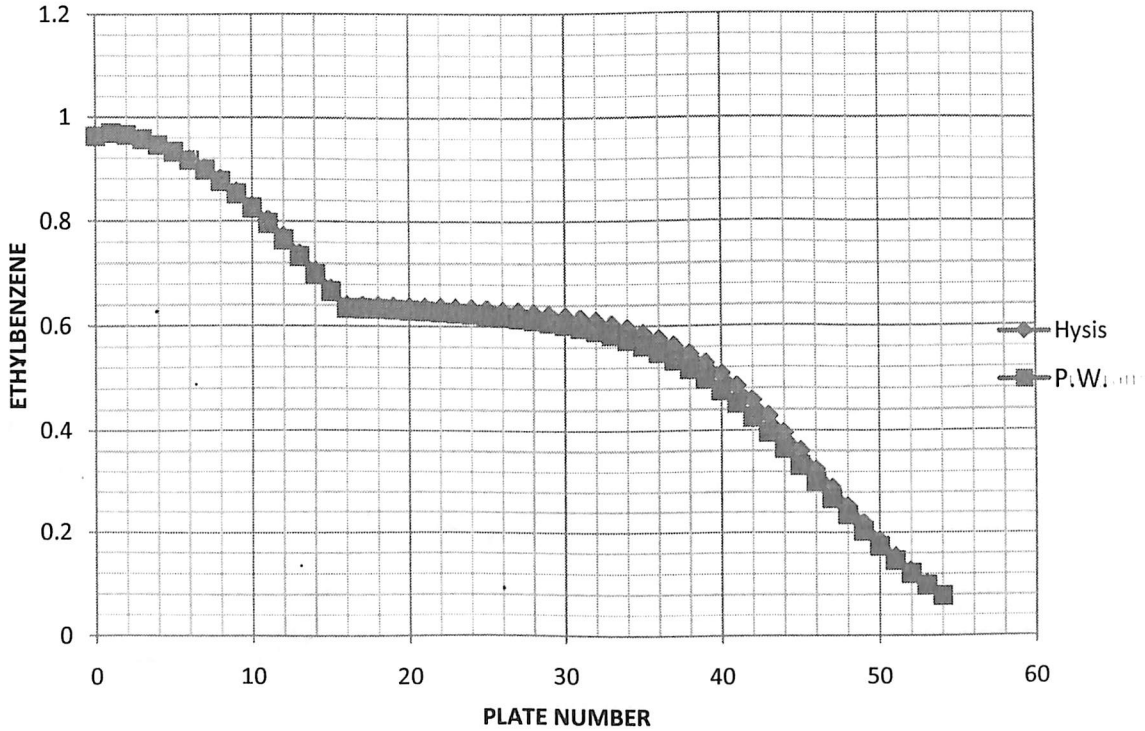

Figure 38: Ethyl Benzene liquid composition profile for the separation of EB - Styrene

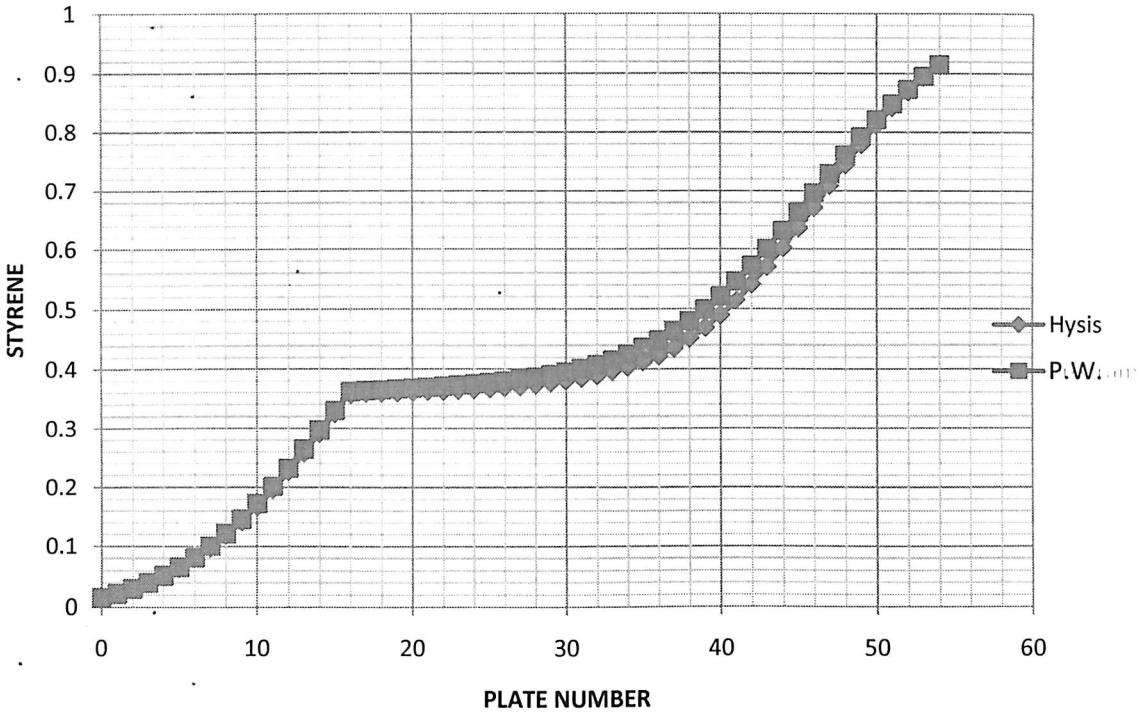

Figure 39: Styrene liquid composition profile for the separation of EB - Styrene

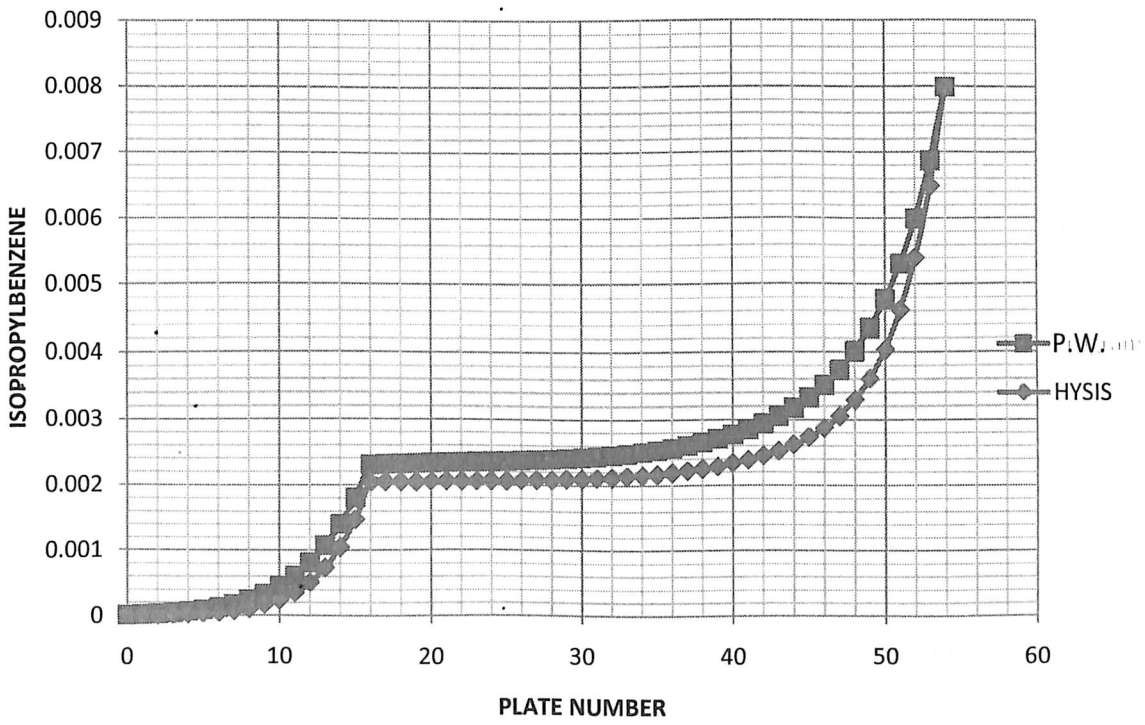

Figure 40: I-propylbenzene liquidcomposition profile for the separation of EB - Styrene

EXAMPLE 07: SEPERATION-OF-TOLUENE_ETHYL-BENZENE

The average deviations in temperature and compositions profiles for toluene-ethylbenzene separation in rectifying and stripping sections are presented in Table-18.

Both the simulations have resulted almost identical temperature profile as shown in Fig-41. There exits very good agreement for the liquid compositions profile of benzene in both the cases of simulations. As shown in Fig-42-45, slightly high composition profiles are found for toluene, ethylbenzene and styrene in the rectifying section and highly compatible profiles in the stripping section.

Table 18: Average deviation in rectifying and stripping section for separation of toluene-ethylbenzene

Separation of toluene-ethyl benzene	T °C		benzene		toluene		ethyl benzene		styrene	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	2.92	0.68	0.002	0.000	0.015	0.001	0.011	0.000	0.006	0.000

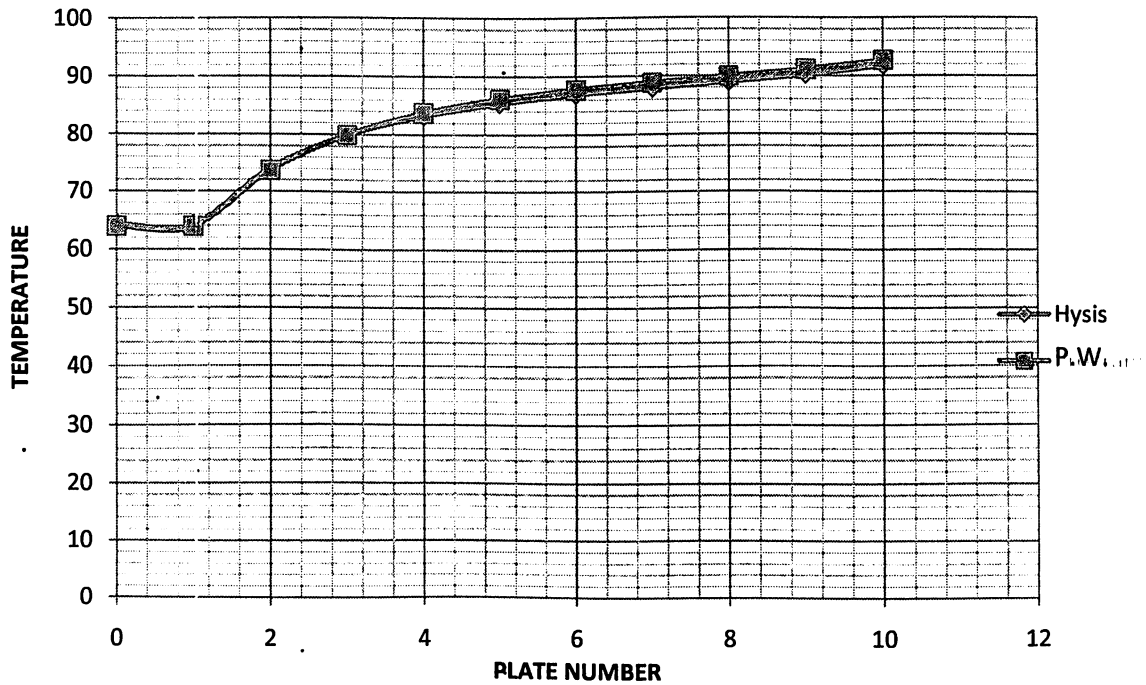

Figure 41: Temperature profile for the separation of Toluene - EB

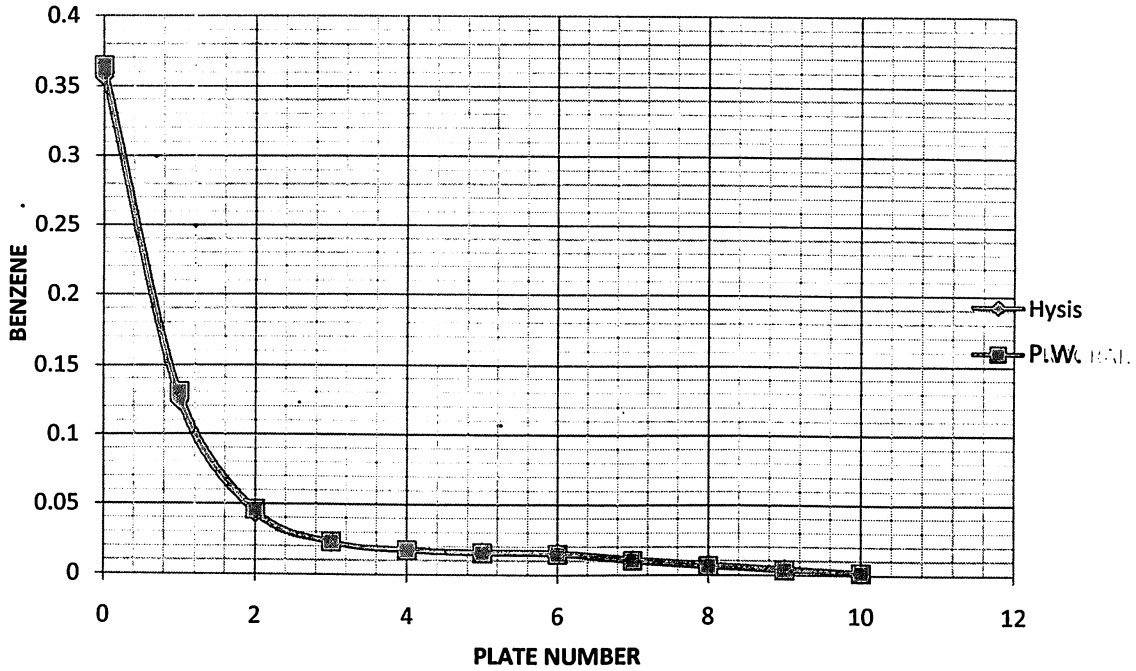

Figure 42: Benzene liquid composition profile for the separation of Toluene - EB

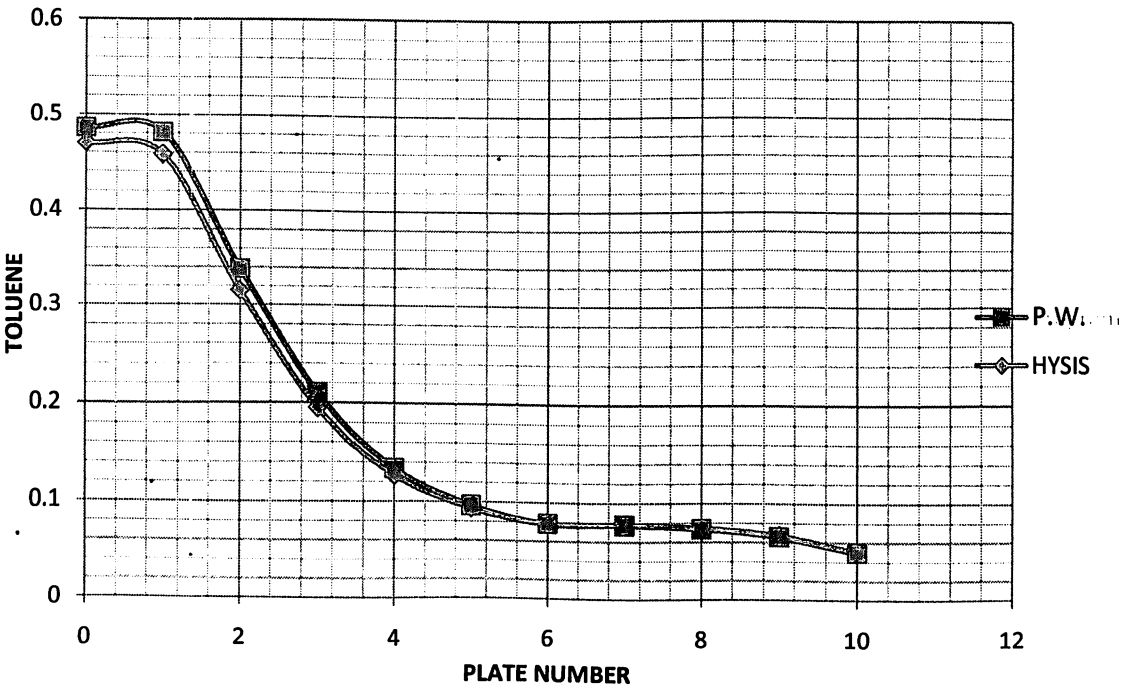

Figure 43: Toluene liquid composition profile for the separation of Toluene - EB

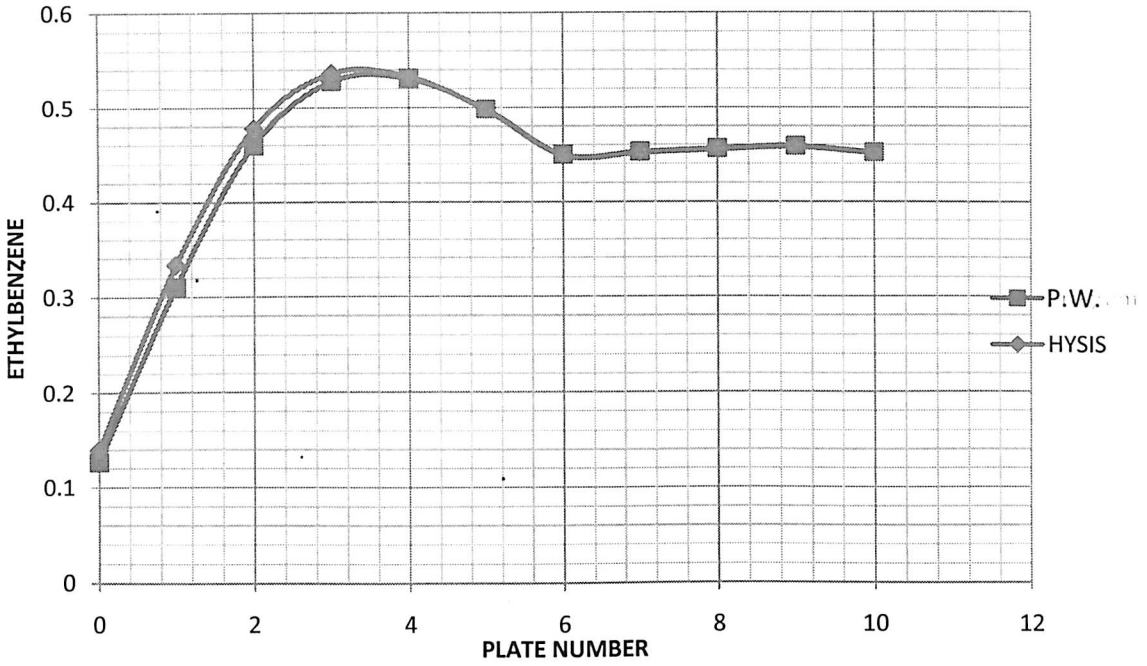

Figure 44: Ethylbenzene liquid composition profile for the separation of Toluene - EB

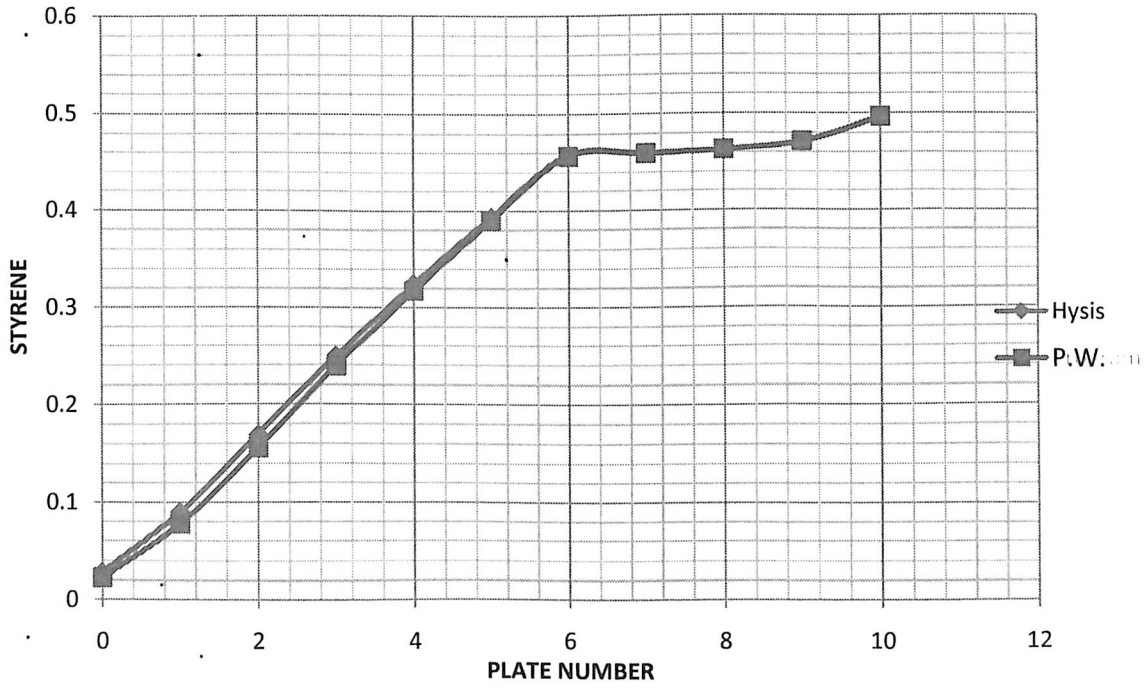

Figure 45: Styrene liquid composition profile for the separation of Toluene - EB

EXAMPLE 08: BIPHENYL-SEPARATION

The biphenyl separation is a typical example for a wide range boiling mixture and while biphenyl concentrates in the stripping section liquid, the temperature profile may increase very steeply posing problems in simulations.

The average deviations in temperature and compositions profiles for biphenyl separation in rectifying and stripping sections are presented in Table-19. As shown in Fig-46 the temperature profile for rectifying section has been predicted in both the simulations of Hysys and present work. For the stripping section the variation is in the range of 4.6 °C. As observed from Fig-47-49There exits very good agreement for the liquid compositions profile of benzene in both the cases of simulations. A little variations in the composition profiles of toluene and diphenyl observed in the stripping section.

Table 19: Average deviation in rectifying and stripping section for biphenyl separation

Biphenyl separation	T °C		benzene		toluene		diphenyl	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	1.16	4.66	0.008	0.007	0.008	0.106	0.000	0.099

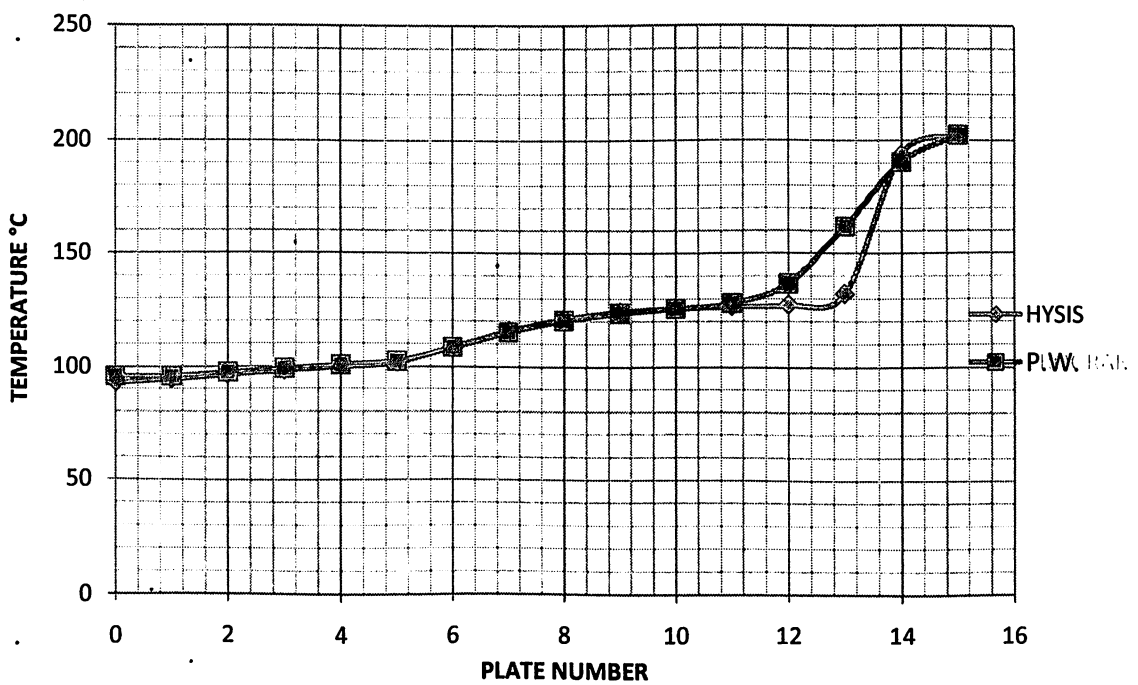

Figure 46: Temperature profile for the Biphenyl separation

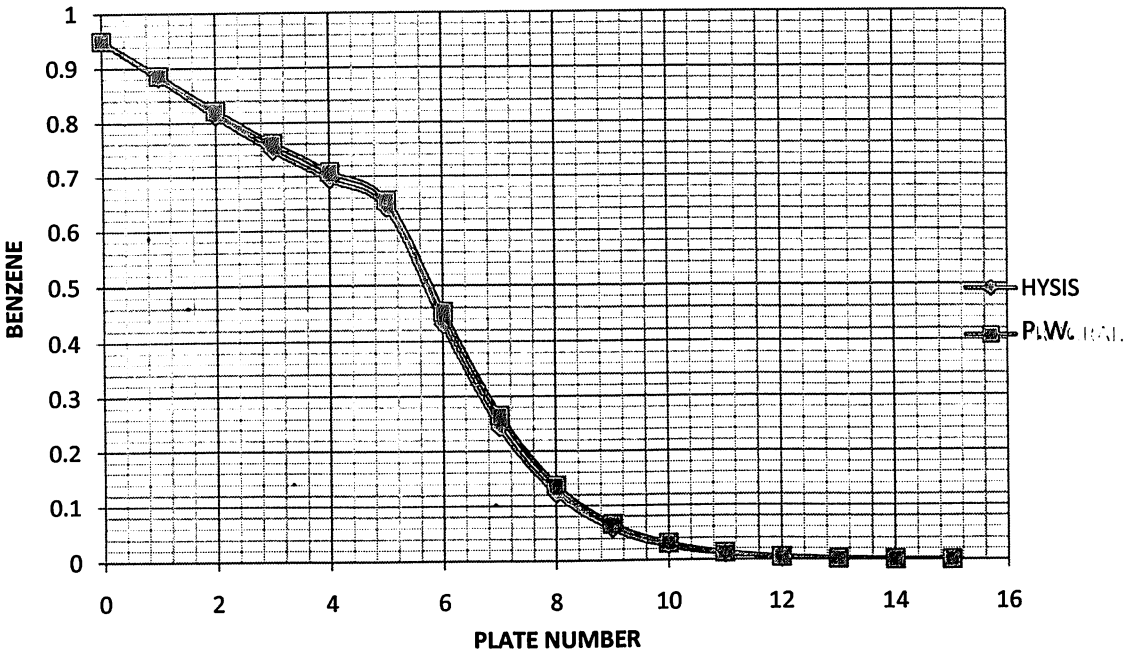

Figure 47: Benzene liquid composition profile for the Biphenyl separation

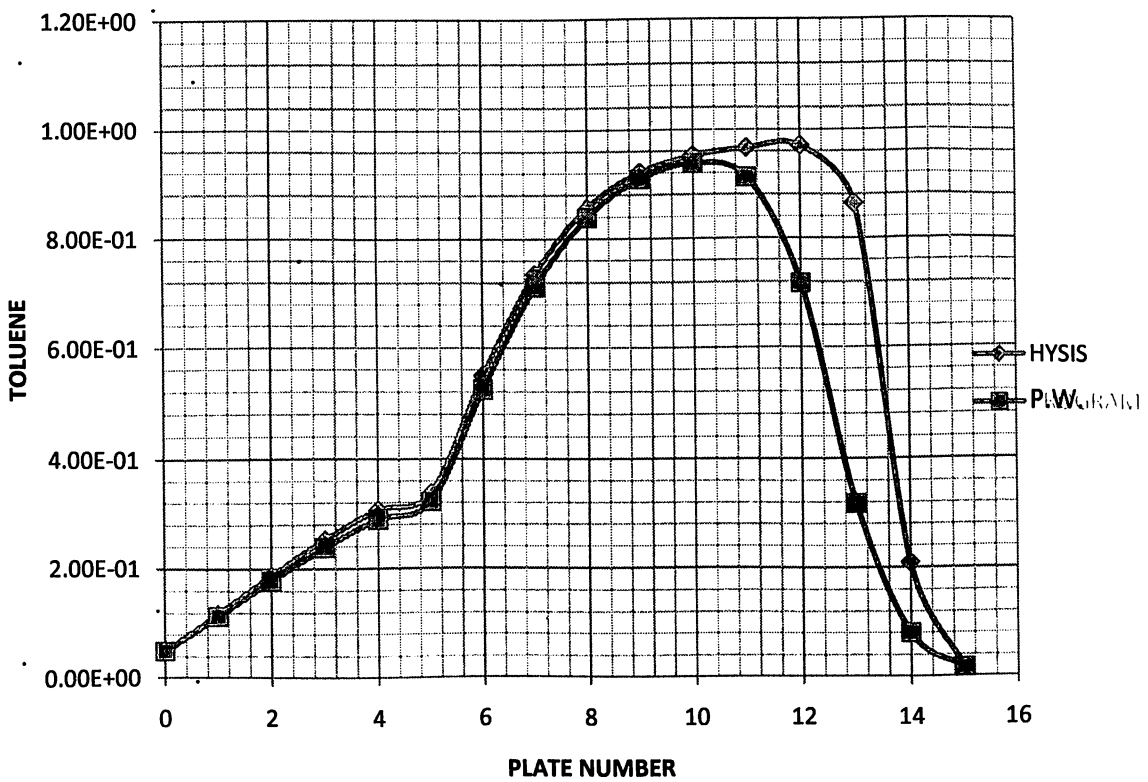

Figure 48: Toluene liquid composition profile for the Biphenyl separation

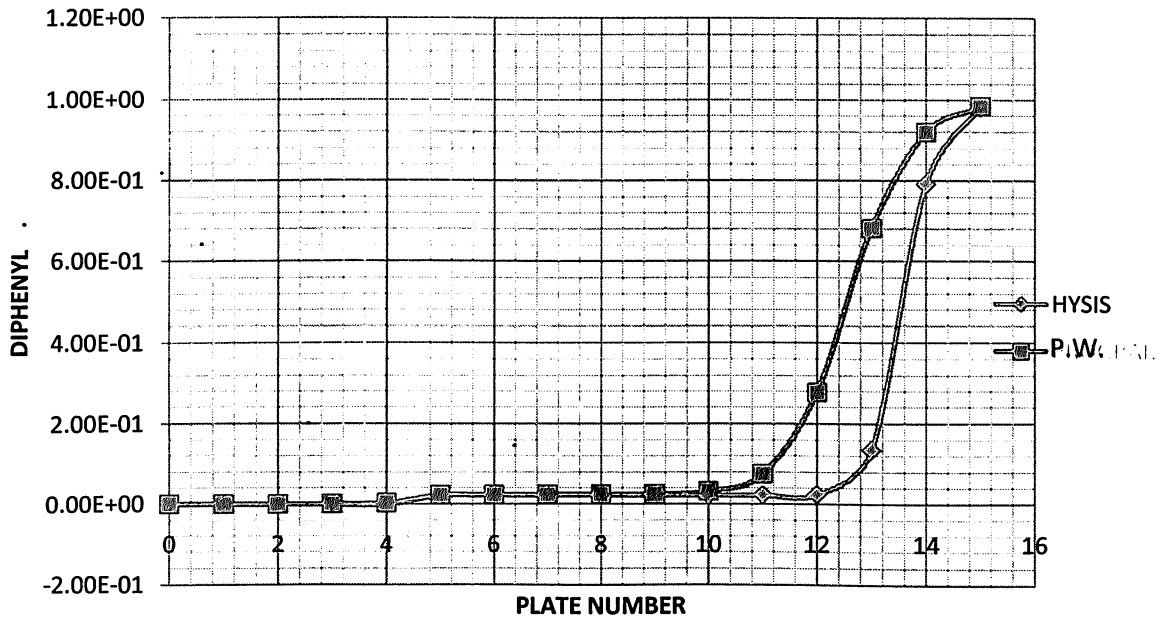

Figure 49: Diphenyl liquid composition profile for the Biphenyl separation

EXAMPLE 9: PHENOL-CRESOL-SEPARATION

This separation is also a standard industrial example used for evaluating column internals for low pressure distillations.

The average deviations in temperature and compositions profiles for phenol-cresol separation in rectifying and stripping sections are presented in Table-20. Both the simulations have resulted almost identical temperature profile as shown in Fig-50. As observed from Fig-51-54, there exits very good agreement for the liquid compositions profile of o-xylene in both the cases of simulations. The liquid composition profiles predicted by the present work for phenol and m-xylene are slightly below the Hysys simulation results, whereas the trend reversed for 2,3 xylenol.

Table 20: Average deviation in rectifying and stripping section for phenol-cresol separation

Phenol-cresol separation	T °C		phenol		o-cresol		m-cresol		2,3-xylenol	
	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S	R.S	S.S
	0.14	0.26	0.003	0.002	0.003	0.002	0.000	0.000	0.000	0.000

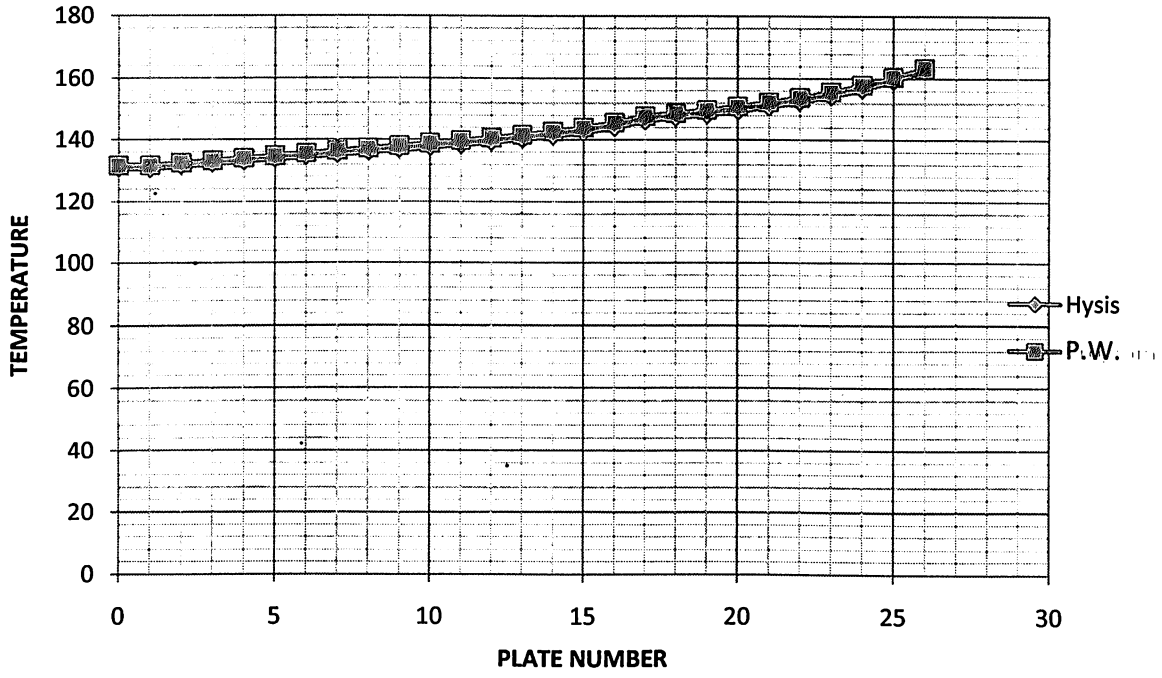

Figure 50: Temperature profile for the Phenol – Cresol separation

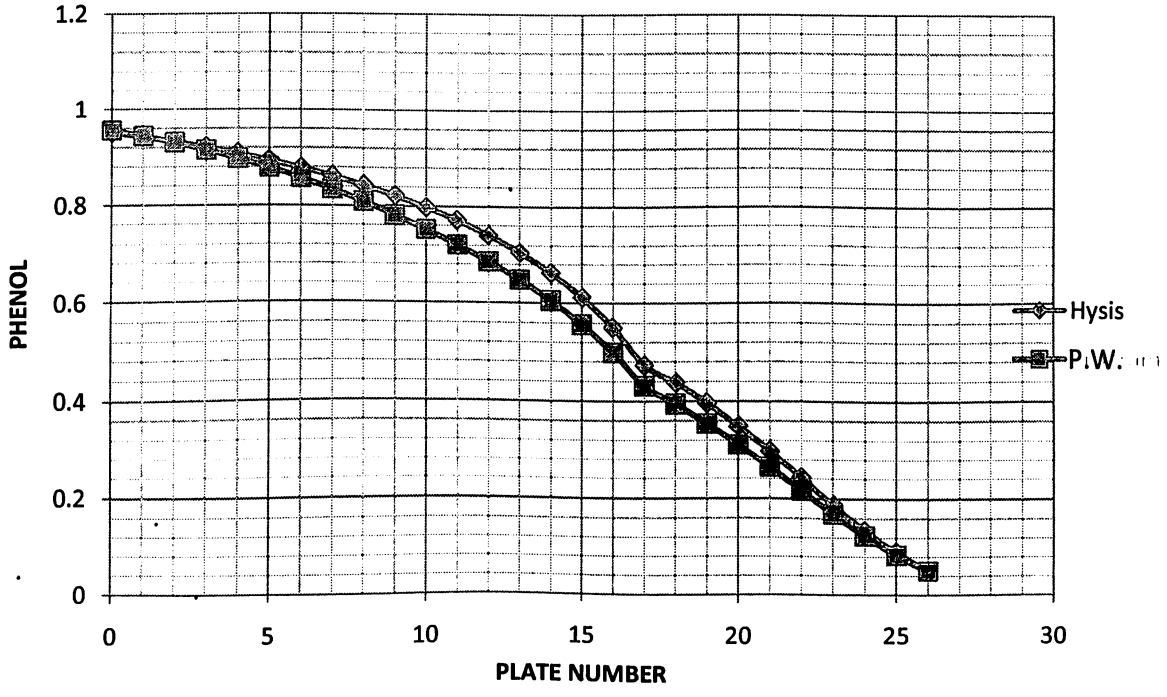

Figure 51: Phenol liquid composition profile for the Phenol – Cresol separation

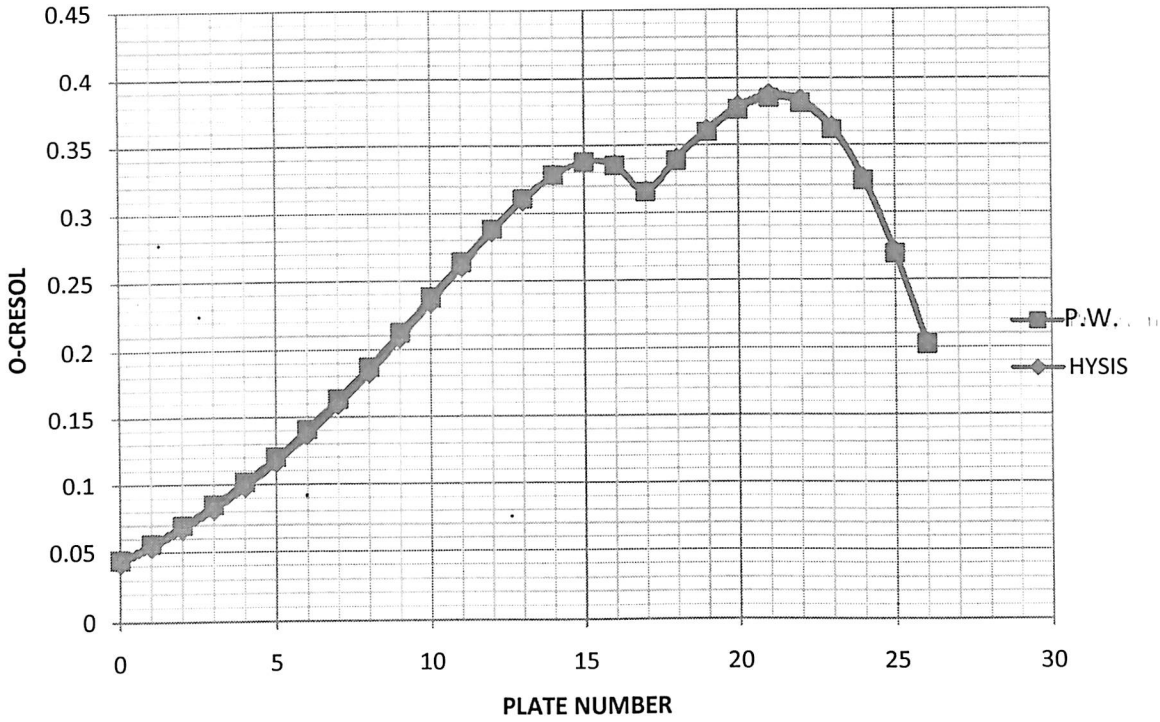

Figure 52: O-cresol liquid composition profile for the Phenol – Cresol separation

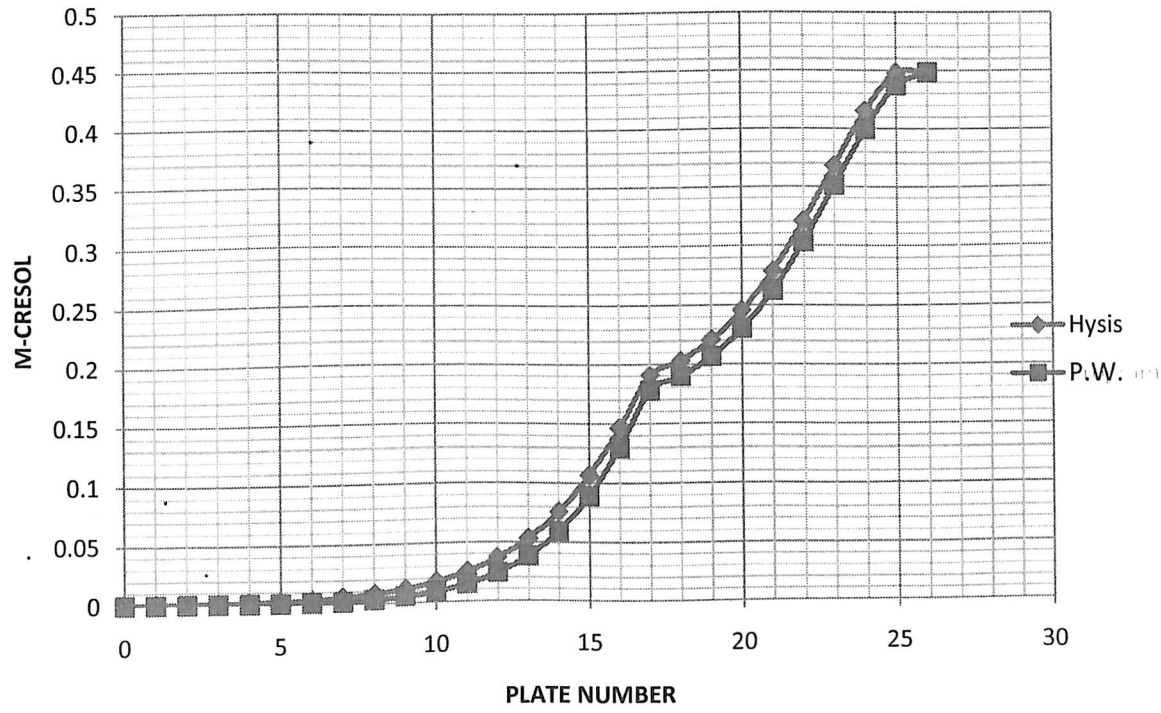

Figure 53: O-cresol liquid composition profile for the Phenol – Cresol separation

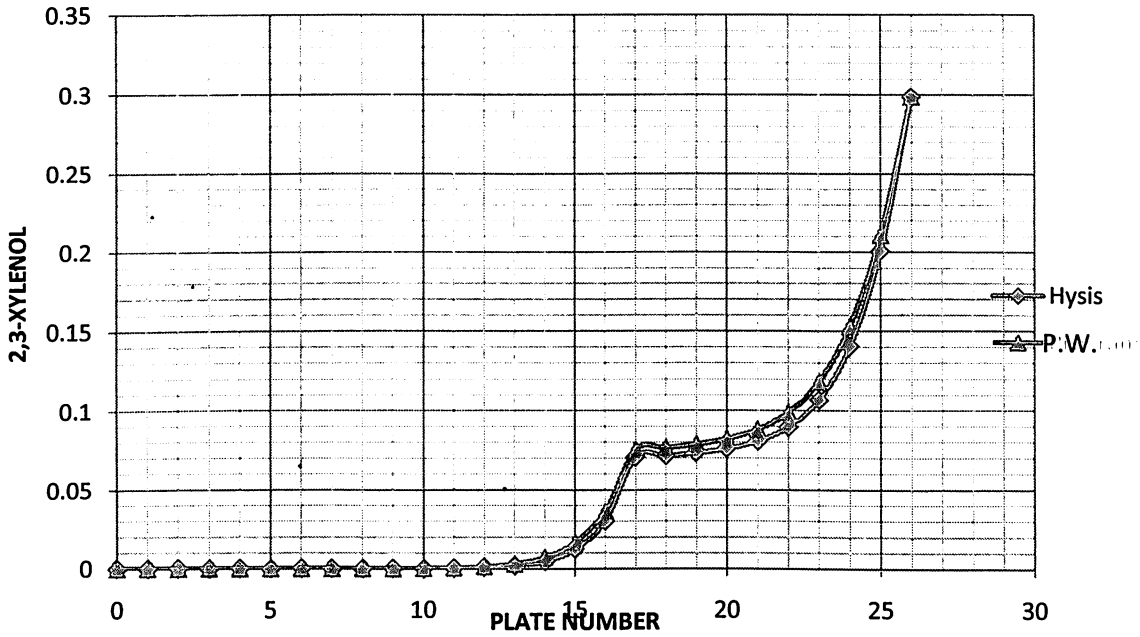

Figure 54: 2,3 – xylenol liquid composition profile for the Phenol – Cresol separation

The deviations observed in the results of Hysys and present work may be attributed to the assumptions of consant phase flow rates in the rectifying and stripping sections of the column.

Though the Antoine constants are used to calculate vaour pressures of components to compute 'K' values for simulations in both the cases, the anoine equations may not be same in Hysis and present work.

5. CONCLUSIONS

1) The development of the Thiele-Geddes (TG) method has been reviewed.

2) A step-wise procedure is given to simulate a distillation column for multicomponent mixtures with an assumption of constant molal flow.

3) Computer programs for four variations of the T-G method to simulate multicomponent distillation columns have been written in 'C++' and the code is presented.

4) Example problems on separations of different liquid mixtures have been used to test the programs and the results are presented.

5) For nearly ideal liquid mixtures, the assumption of constant molal flow is valid as is observed from the good agreement between the simulation results obtained using the programs developed in this work and those of Hysys.

6) These simulation programs are useful to study the optimum feed location and to arrive at the final design parameters for rigorous calculations by adding a subroutine on enthalpy balances.

APPENDIX –I: COMPUTER PROGRAMS

TGXBP

```
//Simulation of a conventional distillation column
//Thiele Geddes method with assumption of Constant Molal Overflow
//Material Balance equations are based on compositions
//Corrections of Temperatures by bp method
//Condenser type: Total
#include<iostream.h>
#include<iomanip.h>
#include<conio.h>
#include<math.h>
#include<fstream.h>
int main()
{
int i,j,iter,NR,NS,NF,NP,NC;
double
F,D,B,R,TTOP,TBOT,PTOP,delp,delt,Q,RL,RV,SL,SV,SUMXD,SUMXB,SUMXD0=1.0,D
SUMXD,SUMY,DSUMY,XF[30],a[30],b[30],c[30],XD[30],XB[30],K[110][30],T[110],PT[1
10],RBD[30],SUMX[110],Y[110][30],X[110][30],RYX[110][30],SXX[110][30],SYX[110][3
0],RXX[110][30];
/*cout<<"enter F, Q, D, R, NC, NR, NS, TTOP, TBOT, PTOP, DELP "<<endl;
cin>>F>>Q>>D>>R>>NC>>NR>>NS>>TTOP>>TBOT>>PTOP>>delp;
cout<<"enter the feed compositions & antonie constants a,b,c"<<endl;
for(i=1;i<=NC;i++)
{  cin>>XF[i]>>a[i]>>b[i]>>c[i];  } */
cout.precision(5);
ofstream amar("TGoutput.txt");
RL=R*D;  RV=RL+D;  SL=RL+Q*F;  B=F-D;  SV=SL-B;  NP=NR+NS+2;  NF=NP-NS-1;
T[1]=TTOP; PT[1]=PTOP;
delt=(TBOT-TTOP)/(NP-1);
for(j=2;j<=NP;j++)
```

```
{ PT[j]=PT[j-1]+delp; T[j]=T[j-1]+delt; }
for(i=1;i<=NC;i++)
{ RYX[1][i]=1; SXX[NP][i]=1; }
for(iter=1;iter<=20;iter++)
{   for(j=1;j<=NP;j++)
      { for(i=1;i<=NC;i++)
        { K[j][i]=exp(a[i]-(b[i]/(c[i]+T[j])))/PT[j]; }
      }
      for(j=1;j<=NR;j++)
      { for(i=1;i<=NC;i++)
        { RXX[j][i]=RYX[j][i]/K[j][i];
          RYX[j+1][i]=(RL*RXX[j][i]+D)/RV;
        }
      }
      for(i=1;i<=NC;i++)
      { SYX[NP][i]=K[NP][i]; }
      for(j=1;j<=NS+1;j++)
      { for(i=1;i<=NC;i++)
        { SXX[NP-j][i]=(SV*SYX[NP-j+1][i]+B)/SL;
          SYX[NP-j][i]=SXX[NP-j][i]*K[NP-j][i];
        }
      }
      for(i=1;i<=NC;i++)
      { RBD[i]=RYX[NF][i]/SYX[NF][i]; }
      SUMXD=0; SUMXB=0;
      for(i=1;i<=NC;i++)
      { XD[i]=F*XF[i]/(D+B*RBD[i]);
        XB[i]=RBD[i]*XD[i];
        SUMXD+=XD[i]; SUMXB+=XB[i];
      }
      for(i=1;i<=NC;i++)
      { XD[i]=XD[i]/SUMXD; XB[i]=XB[i]/SUMXB; }
      for(j=1;j<=NR;j++)
      { for(i=1;i<=NC;i++)
```

```
        { X[j][i]=RXX[j][i]*XD[i]; }
      }
      for(j=0;j<=NS+1;j++)
      { for(i=1;i<=NC;i++)
        { X[NP-j][i]=SXX[NP-j][i]*XB[i]; }
      }
      for(j=1;j<=NP;j++)
      { SUMX[j]=0;
       for(i=1;i<=NC;i++)
       { SUMX[j]+=X[j][i]; }
      }
      for(j=1;j<=NP;j++)
      { for(i=1;i<=NC;i++)
        { X[j][i]=X[j][i]/SUMX[j]; }
      }
      if(fabs(SUMXD-SUMXD0)<=0.00001)      break;
      SUMXD0=SUMXD;
      for(j=1;j<=NP;j++)
      { while(1)
        { SUMY=0; DSUMY=0;
          for(i=1;i<=NC;i++)
          { K[j][i]=exp(a[i]-(b[i]/(c[i]+T[j])))/PT[j];
            Y[j][i]=X[j][i]*K[j][i];
            SUMY+=Y[j][i]; DSUMY+=(b[i]*Y[j][i]/pow((c[i]+T[j]),2));
          } if(fabs(SUMY-1)<=0.000001)   break;
            T[j]=T[j]-((SUMY-1)/DSUMY);
        }
      }
    if(iter>20)break;
}amar<<"sum= "<<SUMXD<<endl;
amar<<"ITERATIONS = "<<iter<<endl;
amar<<endl<<"xD "<<"\t"<<"xB "<<endl;
for(i=1;i<=NC;i++)
{ amar<<XD[i]<<"\t"<<XB[i]<<endl; }
```

```
amar<<endl<<"P.NO "<<"\t"<<"TEMPERATURE "<<"\t"<<"COMPOSITIONS "<<endl;
for(j=1;j<=NP;j++)
{ amar<<j<<"\t"<<(T[j]-273)<<"\t";
        for(i=1;i<=NC;i++)
        { amar<<X[j][i]<<"\t"; }
        amar<<endl;
}
amar.close();
}
```

TGXBPTH

```
//Simulation of a conventional distillation column
//Thiele Geddes method with assumption of Constant Molal Overflow
//Material Balance equations are based on compositions
//Theta convergence method
//Corrections of Temperatures by bp method
//Condensor type: Total
#include<iostream.h>
#include<iomanip.h>
#include<conio.h>
#include<math.h>
#include<fstream.h>
int main()
{
int i,j,l,iter,NR,NS,NF,NP,NC;
double
F,D,B,R,TTOP,TBOT,PTOP,delp,delt,Q,THETA0,THETA,RL,RV,SL,SV,SUMXD,SUMXB
,DSUMXD,DSUMY,SUMY,XF[30],a[30],b[30],c[30],XD[30],XB[30],K[110][30],T[110],P
T[110],RBD[30],SUMX[110],Y[110][30],X[110][30];
double RYX[110][30],SXX[110][30],SYX[110][30],RXX[110][30];
/*cout<<"enter F, Q, D, R, NC, NR, NS, TTOP, TBOT, PTOP, DELP, THETA, THETAO
"<<endl;
```

```
amar<<endl<<"P.NO "<<"\t"<<"TEMPERATURE "<<"\t"<<"COMPOSITIONS "<<endl;
for(j=1;j<=NP;j++)
{ amar<<j<<"\t"<<(T[j]-273)<<"\t";
        for(i=1;i<=NC;i++)
        { amar<<X[j][i]<<"\t"; }
        amar<<endl;
}
amar.close();
}
```

TGXBPTH

```
//Simulation of a conventional distillation column
//Thiele Geddes method with assumption of Constant Molal Overflow
//Material Balance equations are based on compositions
//Theta convergence method
//Corrections of Temperatures by bp method
//Condensor type: Total
#include<iostream.h>
#include<iomanip.h>
#include<conio.h>
#include<math.h>
#include<fstream.h>
int main()
{
int i,j,l,iter,NR,NS,NF,NP,NC;
double
F,D,B,R,TTOP,TBOT,PTOP,delp,delt,Q,THETA0,THETA,RL,RV,SL,SV,SUMXD,SUMXB
,DSUMXD,DSUMY,SUMY,XF[30],a[30],b[30],c[30],XD[30],XB[30],K[110][30],T[110],P
T[110],RBD[30],SUMX[110],Y[110][30],X[110][30];
double RYX[110][30],SXX[110][30],SYX[110][30],RXX[110][30];
/*cout<<"enter F, Q, D, R, NC, NR, NS, TTOP, TBOT, PTOP, DELP, THETA, THETAO
"<<endl;
```

```
cin>>F>>Q>>D>>R>>NC>>NR>>NS>>TTOP>>TBOT>>PTOP>>delp>>THETA>>THET
A0;
cout<<"enter the feed compositions & antonie constants a,b,c"<<endl;
for(i=1;i<=NC;i++)
{ cin>>XF[i]>>a[i]>>b[i]>>c[i]; }*/
cout.precision(5);
ofstream amar("TGTHETAOUTPUT.txt");
RL=R*D; RV=RL+D; SL=RL+Q*F; B=F-D; SV=SL-B; NP=NR+NS+2; NF=NP-NS-1;
T[1]= TTOP; PT[1] = PTOP;
delt=(TBOT-TTOP)/(NP-1);
for(j=2;j<=NP;j++)
{  PT[j]=PT[j-1]+delp; T[j]=T[j-1]+delt; }
for(i=1;i<=NC;i++)
{ RYX[1][i]=1; SXX[NP][i]=1; }
for(iter=1;iter<=30;iter++)
{
      for(j=1;j<=NP;j++)
      { for(i=1;i<=NC;i++)
        { K[j][i]=exp(a[i]-(b[i]/(c[i]+T[j])))/PT[j]; }
      }
      for(j=1;j<=NR;j++)
      { for(i=1;i<=NC;i++)
        { RXX[j][i]=RYX[j][i]/K[j][i];
          RYX[j+1][i]=(RL*RXX[j][i]+D)/RV;
        }
      }
      for(i=1;i<=NC;i++)
      { SYX[NP][i]=K[NP][i]; }
      for(j=1;j<=NS+1;j++)
      { for(i=1;i<=NC;i++)
        { SXX[NP-j][i]=(SV*SYX[NP-j+1][i]+B)/SL;
          SYX[NP-j][i]=SXX[NP-j][i]*K[NP-j][i];
        }
      }
```

```
            for(i=1;i<=NC;i++)
            { RBD[i]=RYX[NF][i]/SYX[NF][i]; }
            for(l=1;l<=500;l++)
            { SUMXD=0; SUMXB=0; DSUMXD=0;
                  for(i=1;i<=NC;i++)
                  { XD[i]=F*XF[i]/(D+B*THETA*RBD[i]);
                    XB[i]=RBD[i]*XD[i];
                    SUMXD+=XD[i]; SUMXB+=XB[i];
                    DSUMXD=DSUMXD-
      (F*XF[i]*B*RBD[i]/pow((D+B*THETA*RBD[i]),2));
                  } if(fabs(SUMXD-1.0)<=0.00001)   break;
                   THETA=THETA-((SUMXD-1)/DSUMXD);
            }
            for(i=1;i<=NC;i++)
            { XD[i]=XD[i]/SUMXD; XB[i]=XB[i]/SUMXB; }
      //CALCULATION OF LIQUID COMPOSITIONS
        for(j=1;j<=NR;j++)
            { for(i=1;i<=NC;i++)
              { X[j][i]=RXX[j][i]*XD[i]; }
            }
            for(j=0;j<=NS+1;j++)
            { for(i=1;i<=NC;i++)
              { X[NP-j][i]=SXX[NP-j][i]*XB[i]; }
            }
            for(j=1;j<=NP;j++)
            { SUMX[j]=0;
                  for(i=1;i<=NC;i++)
                  { SUMX[j]+=X[j][i]; }
            }
            for(j=1;j<=NP;j++)
            { for(i=1;i<=NC;i++)
              { X[j][i]=X[j][i]/SUMX[j]; }
            }
      //CHECK OLD AND NEW VALUES OF THETA
```

```
        if(fabs(THETA-THETA0)<=0.00001)        break;
        THETA0=THETA;
    //CORRECTION OF TEMPERATURE PROFILE
        for(j=1;j<=NP;j++)
        { while(1)
          { SUMY=0; DSUMY=0;
            for(i=1;i<=NC;i++)
            { K[j][i]=exp(a[i]-(b[i]/(c[i]+T[j])))/PT[j];
              Y[j][i]=X[j][i]*K[j][i];
              SUMY+=Y[j][i]; DSUMY+=(b[i]*Y[j][i]/pow((c[i]+T[j]),2));
            } if(fabs(SUMY-1)<=0.00001)    break;
              T[j]=T[j]-((SUMY-1)/DSUMY);
          }
        }
    }
    amar<<"ITERATIONS = "<<iter<<"\t"<<"THETA = "<<THETA<<endl;
    amar<<endl<<"xD "<<"\t"<<"xB "<<endl;
    for(i=1;i<=NC;i++)
    { amar<<XD[i]<<"\t"<<XB[i]<<endl; }
    amar<<endl<<"P.NO "<<"\t"<<"TEMPERATURE "<<"\t"<<"COMPOSITIONS "<<endl;
    for(j=1;j<=NP;j++)
    { amar<<j<<"\t"<<T[j]<<"\t";
        for(i=1;i<=NC;i++)
        { amar<<X[j][i]<<"\t"; }
        amar<<endl;
    }
    amar.close();
    }
```

TGXKBTH

```
//Simulation of a conventional distillation column
//Thiele Geddes method with assumption of Constant Molal Overflow
//Material Balance equations are based on compositions
//Theta convergence method
//Corrections of Temperatures by KB Method
//Condensor type: Total
#include<iostream.h>
#include<iomanip.h>
#include<conio.h>
#include<math.h>
#include<fstream.h>
int main()
{
int i,j,l,iter,NR,NS,NF,NP,NC,NB;
double
F,D,B,R,TTOP,TBOT,PTOP,delp,delt,Q,THETA0,THETA,RL,RV,SL,SV,SUMXD,SUMXB
,DSUMXD;
double
ALFA[110][30],SUMALFX[110],XF[30],a[30],b[30],c[30],XD[30],XB[30],K[110][30],T[11
0],PT[110],RBD[30],SUMX[110],Y[110][30],X[110][30],RYX[110][30],SXX[110][30],SY
X[110][30],RXX[110][30];
/*cout<<"enter F, Q, D, R, NC, NR, NS, TTOP, TBOT, PTOP, DELP, THETA, THETAO,
NB "<<endl;
cin>>F>>Q>>D>>R>>NC>>NR>>NS>>TTOP>>TBOT>>PTOP>>delp>>THETA>>THET
A0>>NB;
cout<<"enter the feed compositions & antonie constants a,b,c"<<endl;
for(i=1;i<=NC;i++)
{ cin>>XF[i]>>a[i]>>b[i]>>c[i]; }*/
cout.precision(5);
ofstream amar("TGKBOUTPUT.txt");
```

```
RL=R*D; RV=RL+D; SL=RL+Q*F; B=F-D; SV=SL-B; NP=NR+NS+2; NF=NP-NS-1;
T[1]=TTOP; PT[1]=PTOP;
delt=(TBOT-TTOP)/(NP-1);
for(j=2;j<=NP;j++)
{ PT[j]=PT[j-1]+delp; T[j]=T[j-1]+delt; }
for(i=1;i<=NC;i++)
{ RYX[1][i]=1; SXX[NP][i]=1; }
for(iter=1;iter<=30;iter++)
{
        for(j=1;j<=NP;j++)
        { for(i=1;i<=NC;i++)
          { K[j][i]=exp(a[i]-(b[i]/(c[i]+T[j])))/PT[j]; }
        }
        for(j=1;j<=NR;j++)
        { for(i=1;i<=NC;i++)
          { RXX[j][i]=RYX[j][i]/K[j][i];
            RYX[j+1][i]=(RL*RXX[j][i]+D)/RV;
          }
        }
        for(i=1;i<=NC;i++)
        { SYX[NP][i]=K[NP][i]; }
        for(j=1;j<=NS+1;j++)
        { for(i=1;i<=NC;i++)
          { SXX[NP-j][i]=(SV*SYX[NP-j+1][i]+B)/SL;
            SYX[NP-j][i]=SXX[NP-j][i]*K[NP-j][i];
          }
        }
        for(i=1;i<=NC;i++)
        { RBD[i]=RYX[NF][i]/SYX[NF][i]; }
        while(1)
        { SUMXD=0; SUMXB=0; DSUMXD=0;
                for(i=1;i<=NC;i++)
                { XD[i]=F*XF[i]/(D+B*THETA*RBD[i]);
                  XB[i]=RBD[i]*XD[i];
```

```
                SUMXD+=XD[i]; SUMXB+=XB[i];
                DSUMXD=DSUMXD-
F*XF[i]*B*RBD[i]/pow((D+B*THETA*RBD[i]),2));
              } if(fabs(SUMXD-1)<=0.000001)   break;
              THETA=THETA-((SUMXD-1)/DSUMXD);
        }
        for(i=1;i<=NC;i++)
  { XD[i]=XD[i]/SUMXD; XB[i]=XB[i]/SUMXB; }
        for(j=1;j<=NR;j++)
        { for(i=1;i<=NC;i++)
          { X[j][i]=RXX[j][i]*XD[i]; }
        }
        for(j=0;j<=NS+1;j++)
        { for(i=1;i<=NC;i++)
          { X[NP-j][i]=SXX[NP-j][i]*XB[i]; }
        }
        for(j=1;j<=NP;j++)
        { SUMX[j]=0;
              for(i=1;i<=NC;i++)
              { SUMX[j]+=X[j][i]; }
        }
        for(j=1;j<=NP;j++)
        { for(i=1;i<=NC;i++)
          { X[j][i]=X[j][i]/SUMX[j]; }
        }
        if(fabs(THETA-THETA0)<=0.000001)      break;
        THETA0=THETA;
        for(j=1;j<=NP;j++)
        { SUMALFX[j]=0;
         for(i=1;i<=NC;i++)
         { ALFA[j][i]=K[j][i]/K[j][NB];
          SUMALFX[j]+=ALFA[j][i] * X[j][i];
         } K[j][NB]=1/SUMALFX[j];
          T[j]=(b[NB]/(a[NB]-log(K[j][NB]*PT[j])))-c[NB];
```

```
        }
    }
    amar<<"ITERATIONS = "<<iter<<"\t"<<"THETA = "<<THETA<<endl;
    amar<<endl<<"xD "<<"\t"<<"xB "<<endl;
    for(i=1;i<=NC;i++)
    { amar<<XD[i]<<"\t"<<XB[i]<<endl; }
    amar<<endl<<"P.NO "<<"\t"<<"TEMPERATURE "<<"\t"<<"COMPOSITIONS "<<endl;
    for(j=1;j<=NP;j++)
    { amar<<j<<"\t"<<(T[j]-273)<<"\t";
        for(i=1;i<=NC;i++)
        { amar<<X[j][i]<<"\t"; }
        amar<<endl;
    } amar.close();
    }
```

TGCKBTTH

```
// Simulation of a conventional distillation column
//Thiele and Geddes Method with assumption of constant molal overflow
// Component molal flow rates are used in the material balance equations
//Thomas algorithm for solving Tridiagonal matrix of material balance equations
//Correction of temperature by kb method
// theta convergence method
//Partial reboiler
//Condenser: Total/partial
#include<iostream.h>
#include<iomanip.h>
#include<math.h>
#include<conio.h>
#include<fstream.h>
int main()
{
int NC,NR,NS,ITER,COND,NT,NF,NB,I,J,XX;
```

```
double
a[20],b[20],c[20],T[100],PT[100],A[20][100],CV[20][100],CLD[20][100],XF[20],XB[20],X
D[20],RBD[20];
double
K[20][100],CD[20],CB[20],SUMALFX[100],ALFA[20][100],X[20][100],SUMCL[100],CL[
20][100];
double F[20][100],M[20][100],G[20][201],TOLD[100],FEED,SUMCD,SUMCB,DSUMCD;
dqube Q,D,R,TTOP,TBOT,PTOP,DELP,THETA,THETAO,B,RV,RL,SL,SV,DELT;
/*cout<<"enter FEED, Q, D, R, NC, NR, NS, TTOP, TBOT, PTOP, DELP, THETA,
THETAO, NB,IF CONDENCER TOTAL ENTER 0"<<endl;
cin>>FEED>>Q>>D>>R>>NC>>NR>>NS>>TTOP>>TBOT>>PTOP>>DELP>>THETA>
>THETA0>>NB>>COND;
cout<<"enter the feed compositions & antonie constants a,b,c"<<endl;
for(i=1;i<=NC;i++)
{ cin>>XF[i]>>a[I]>>b[I]>>c[I]; }*/
cout.precision(5);
ofstream amar("TDMOUTPUT.txt");
B=FEED-D;  RV=D*(R+1);  RL=D*R;  SL=RL+Q*FEED;  SV=RV-(1-Q)*FEED;
NT=NR+NS+2; NF=NT-NS-1; T[2]=TTOP; PT[2]=PTOP;
DELT=(TBOT-TTOP)/(NT-2); PT[1]=PT[2]-DELP;
if(COND==0) T[1]=T[2];
else T[1]=T[2]-DELT;
for(J=3;J<=NT;J++)
{ T[J]=T[J-1]+DELT;
 PT[J]=PT[J-1]+DELP;
}
for(ITER=1;ITER<=30;ITER++)
{
  if(COND>0) XX=1; else XX=2;
  for(J=XX;J<=NT;J++)
  { for(I=1;I<=NC;I++)
    { K[I][J]=exp(a[I]-b[I]/(T[J]+c[I]))/PT[J]; }
  }
  if(COND>0)
```

```
for(I=1;I<=NC;I++)
A[I][1]=RL/(K[I][1]*D);
else
for(I=1;I<=NC;I++)
A[I][1]=RL/D;
for(I=1;I<=NC;I++)
A[I][NT]=B/(K[I][NT]*SV);
for(J=2;J<=NR;J++)
{ for(I=1;I<=NC;I++)
  { A[I][J]=RL/(K[I][J]*RV); }
}
for(I=1;I<=NC;I++)
A[I][NF]=SL/(K[I][NF]*RV);
for(J=NF+1;J<=NT-1;J++)
{ for(I=1;I<=NC;I++)
  { A[I][J]=SL/(K[I][J]*SV); }
}
//THOMAS ALGORITHM
for(I=1;I<=NC;I++)
M[I][0]=1;
for(J=1;J<=NT;J++)
{ for(I=1;I<=NC;I++)
  { M[I][J]=1+A[I][J]*M[I][J-1];
    F[I][J]=-1*M[I][J-1]/M[I][J];
  }
}
for(J=1;J<=NF-2;J++)
{ for(I=1;I<=NC;I++)
  { G[I][J]=0; }
}
for(I=1;I<=NC;I++)
{ G[I][NF-1]=(1-Q)*FEED*XF[I]*M[I][NF-2]/M[I][NF-1];
  G[I][NF]=(FEED*Q*XF[I]+A[I][NF-1]*G[I][NF-1])*M[I][NF-1]/M[I][NF];
}
```

```
for(J=NF+1;J<=NT;J++)
{ for(I=1;I<=NC;I++)
  { G[I][J]=A[I][J-1]*G[I][J-1]*M[I][J-1]/M[I][J]; }
}
for(I=1;I<=NC;I++)
CV[I][NT]=G[I][NT];
for(J=1;J<=NT-1;J++)
{ for(I=1;I<=NC;I++)
  { CV[I][NT-J]=G[I][NT-J]-F[I][NT-J]*CV[I][NT-J+1]; }
}
for(I=1;I<=NC;I++)
{ CD[I]=CV[I][1];
  CB[I]=A[I][NT]*CV[I][NT];
  RBD[I]=CB[I]/CD[I];
}
for(J=2;J<=NT;J++)
{ for(I=1;I<=NC;I++)
  { CLD[I][J]=A[I][J]*CV[I][J]/CD[I]; }
}
while(1)
{ SUMCD=0.0; SUMCB=0.0; DSUMCD=0.0;
  for(I=1;I<=NC;I++)
  { CD[I]=FEED*XF[I]/(1+THETA*RBD[I]);
    CB[I]=CD[I]*RBD[I];
    SUMCD=SUMCD+CD[I]; SUMCB=SUMCB+CB[I];
    DSUMCD=DSUMCD-FEED*XF[I]*RBD[I]/pow(1+THETA*RBD[I],2);
  }
  for(I=1;I<=NC;I++)
  { XD[I]=CD[I]/SUMCD; XB[I]=CB[I]/SUMCB; }
  if(fabs(SUMCD/D-1)<pow(10,-6)) break;
  THETA=THETA-(SUMCD-D)/DSUMCD;
}//End of while()
for(J=2;J<=NT;J++)
{ for(I=1;I<=NC;I++)
```

```
        { CL[I][J]=CLD[I][J]*CD[I]; }
       }
       for(I=1;I<=NC;I++)
       CL[I][1]=A[I][1]*CD[I];
     //CALCULATION OF LIQUID COMPOSITIONS
       for(J=1;J<=NT;J++)
       { SUMCL[J]=0;
        for(I=1;I<=NC;I++)
        SUMCL[J]=SUMCL[J]+CL[I][J];
       }
       for(J=1;J<=NT;J++)
       { for(I=1;I<=NC;I++)
        { X[I][J]=CL[I][J]/SUMCL[J]; }
       }
    //CHECK OLD AND NEW VALUES OF THETA
      if(fabs(THETA-THETAO)<=0.00001)  break;
      THETAO=THETA;
    //CORRECTION OF TEMPERATURE PROFILE
      for(J=1;J<=NT;J++)
          { SUMALFX[J]=0;
           for(I=1;I<=NC;I++)
           { ALFA[I][J]=K[I][J]/K[NB][J];
            SUMALFX[J]+=ALFA[I][J] * X[I][J];
           } K[NB][J]=1/SUMALFX[J];
            T[J]=(b[NB]/(a[NB]-log(K[NB][J]*PT[J])))-c[NB];
        }}
amar<<"ITERATIONS = "<<ITER<<"\t"<<"THETA = "<<THETA<<endl;
amar<<"xD"<<"\t"<<"xB"<<endl;
for(I=1;I<=NC;I++)
{ amar<<XD[I]<<"\t"<<XB[I]<<endl; }
amar<<"P.NO "<<"\t"<<"TEMPERATURE "<<"\t"<<"COMPOSITIONS "<<endl;
for(J=1;J<=NT;J++)
{ amar<<J<<"\t"<<T[J]<<"\t";
       for(I=1;I<=NC;I++)
```

```
            { amar<<X[I][J]<<"\t"; }
            amar<<endl;
        } amar.close();}
```

APPENDIX-II: INPUT DATA

EXAMPLE 1

DEPROPANIZER-I

Feed Rate, F: 349.4 moles/hr

Feed Composition, x_{iF}: ethane 0.006868; propane 0.465940; i-butane 0.088720; n-butane 0.219520; n-pentane 0.218950;

Feed Enthalpy, Q=1

Distillate Rate, D=165.2 moles/hr

Reflux Ratio, R=1.737

Theoretical Plates in Rectifying Section, NR=9

Theoretical Plates in Stripping Section, NS=10

Pressure Drop per Plate=5 mm Hg

Pressure in the Condenser, PT=16290.203 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 2

SEPARATION OF PARAFFINS

Feed Rate, F: 1.0 moles/hr

Feed Composition, x_{iF}: nonane 0.026; n-decane 0.224; undecane 0.235; n-dodacane 0.192; n-tridecane 0.186; n-tetradecane 0.137;

Feed Enthalpy, Q=1

Distillate Rate, D=0.1 moles/hr

Reflux Ratio, R=1.0

Theoretical Plates in Rectifying Section, NR=10

Theoretical Plates in Stripping Section, NS=10

Pressure Drop per Plate=5 mm Hg

Pressure in the Condenser, PT=530 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 3

DEPROPANIZER-II

Feed Rate, F: 100.0 moles/hr

Feed Composition, x_{iF}: methane 0.26; ethane 0.09; propane 0.25; n-butane 0.17; n-pentane 0.11; n-hexane 0.12

Feed Enthalpy, Q=1

Distillate Rate, D=59.9 moles/hr

Reflux Ratio, R=1.5

Theoretical Plates in Rectifying Section, NR=9

Theoretical Plates in Stripping Section, NS=9

Pressure Drop per Plate=4 mm Hg

Pressure in the Condenser, PT=16285.7 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 4

ETHANE-SPLITTER

Feed Rate, F: 100.0 moles/hr

Feed Composition, x_{iF}: methane 0.05; mthane 0.35; propylene 0.15; propane 0.10; i-butane 0.10; n-butane 0.15

Feed Enthalpy, Q=1

Distillate Rate, D=38.5 moles/hr

Reflux Ratio, R=1.722

Theoretical Plates in Rectifying Section, NR=6

Theoretical Plates in Stripping Section, NS=6

Pressure Drop per Plate=5 mm Hg

Pressure in the Condenser, PT=20679.6 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 5

FRACTIONATION OF XYLENES

Feed Rate, F: 250.0 moles/hr

Feed Composition, x_{iF}: ethylbenzane 0.050; p-xylene 0.565; m-xylene 0.190; o-xylene 0.195

Feed Enthalpy, Q=1

Distillate Rate, D=205 moles/hr

Reflux Ratio, R=10.5

Theoretical Plates in Rectifying Section, NR=45

Theoretical Plates in Stripping Section, NS=53

Pressure Drop per Plate=3 mm Hg

Pressure in the Condenser, PT=760 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 6

ETHYLBENZENE-STYRENE SEPARATION

Feed Rate, F: 38.0 moles/hr

Feed Composition, x_{iF}: toluene 0.011; ethylbenzane 0.520; styrene 0.465; i-propylbenzene 0.004

Feed Enthalpy, Q=1

Distillate Rate, D=19.0 moles/hr

Reflux Ratio, R=7.0

Theoretical Plates in Rectifying Section, NR=15

Theoretical Plates in Stripping Section, NS=37

Pressure Drop per Plate=3 mm Hg

Pressure in the Condenser, PT=50 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 7

SEPERATION OF TOLUENE-ETHYL BENZENE

Feed Rate, F: 100.0 moles/hr

Feed Composition, x_{iF}: benzene 0.022;toluene 0.074; ethylbenzane 0.434; styrene 0.470;

Feed Enthalpy, Q=1

Distillate Rate, D=5.58 moles/hr

Reflux Ratio, R=4.36

Theoretical Plates in Rectifying Section, NR=5

Theoretical Plates in Stripping Section, NS=3

Pressure Drop per Plate=3 mm Hg

Pressure in the Condenser, PT=160 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 8

BIPHENYL-SEPARATION

Feed Rate, F: 1.0 moles/hr

Feed Composition, x_{iF}: benzene 0.022; toluene 0.074; ethylbenzane 0.434; styrene 0.470;

Feed Enthalpy, Q=1

Distillate Rate, D=0.959 moles/hr

Reflux Ratio, R=1.0

Theoretical Plates in Rectifying Section, NR=4

Theoretical Plates in Stripping Section, NS=9

Pressure Drop per Plate=4 mm Hg

Pressure in the Condenser, PT=1122 mm Hg

Total Condenser and Partial Rebolier

EXAMPLE 9

PHENOL-CRESOL-SEPARATION

Feed Rate, F: 100.0 moles/hr

Feed Composition, x_{iF}: phenol 0.35; o-cresol 0.15; m-cresol 0.30; 2,3-xylenol 0.20;

Feed Enthalpy, Q=1

Distillate Rate, D=33.1 moles/hr

Reflux Ratio, R=10.0

Theoretical Plates in Rectifying Section, NR=16

Theoretical Plates in Stripping Section, NS=8

Pressure Drop per Plate=4 mm Hg

Pressure in the Condenser, PT=150 mm Hg

Total Condenser and Partial Rebolier

Table - 21 Antoine constants data

Component	A	B	C
Methane	15.2243	897.84	-7.16
Ethane	15.6637	1511.42	-17.16
Propane	15.7260	1872.46	-25.16
Propylene	15.7027	1807.46	-26.15
n-butane	15.6782	2154.90	-34.42
i-butane	15.5381	2032.73	-33.15
n-pentane	15.8333	2477.07	-39.94
n-hexane	15.8366	2697.55	-48.78
Nonane	15.9670	3291.453	-71.330
n-decane	16.034	3474.025	-77.776
Undecane	16.0541	3614.068	-85.450
n-dodacane	16.1134	3774.559	-91.315
n-tridecane	16.1355	3892.912	-98.930
n-tetradecane	16.1480	4008.524	-105.43
Benzene	15.9008	2788.51	-52.36
Toluene	16.0137	3096.52	-53.67
ethyl benzene	16.0195	3279.47	-59.95
Styrene	16.0193	3328.57	-63.72
1,4 diethyl benzene	16.1140	3657.22	-71.18
i-propyl benzene	15.9722	3363.60	-63.37
Biphenyl	16.6832	4602.23	-70.42
Phenol	16.4279	3490.89	-98.59
o-cresol	15.9148	3305.37	-108.0
m-cresol	17.2878	4274.42	-74.09
Xylenol	16.2424	3724.58	-102.4

The Antoine constants for the components in the above problems are taken from Reid et al.[30] to calculate the pure component vapour pressures required to compute K values.

APPENDIX-III: OUTPUT DATA

TGXBP

Example 01

Depropanizer

Sum xD = 1.00468; Iterations = 20

Component	xD	xB
ethane	0.0144582	3.87905e-011
propane	0.979996	0.000796653
i-butane	0.0049781	0.164494
n-butane	0.000567841	0.41764
n-pentane	1.41583e-008	0.417068

Plate number	T °C	Liquid Compositions				
		ethane	propane	i-butane	n-butane	n-pentane
1	62.5528	0.00426614	0.981912	0.0119872	0.00183416	1.33012e-007
2	63.2134	0.00233543	0.970927	0.0223746	0.00436229	8.2624e-007
3	63.9193	0.00195765	0.951284	0.0374423	0.00931097	4.78837e-006
4	64.9526	0.00186078	0.920968	0.0584628	0.0186812	2.67434e-005
5	66.5077	0.00180302	0.876518	0.0859991	0.0355366	0.000142854
6	68.769	0.00173654	0.815189	0.118704	0.0636537	0.000717006
7	71.8824	0.00165194	0.73714	0.152054	0.105846	0.00330905
8	75.973	0.00154887	0.646173	0.178077	0.160487	0.0137145
9	81.4371	0.00142494	0.546361	0.186459	0.216291	0.049464
10	89.4976	0.00126798	0.437915	0.167175	0.247029	0.146613
11	95.0983	0.0003398	0.348892	0.21161	0.286974	0.152184
12	101.749	8.412e-005	0.250669	0.257928	0.33284	0.158479
13	108.318	1.930e-005	0.163236	0.29576	0.376685	0.1643
14	113.715	4.173e-006	0.0982971	0.319372	0.413396	0.16893

15	117.57	8.652e-007	0.0560254	0.328897	0.442568	0.172509
16	120.135	1.745e-007	0.030772	0.32705	0.466252	0.175926
17	121.896	3.457e-008	0.0164475	0.316215	0.486263	0.181075
18	123.39	6.741e-009	0.00856027	0.297115	0.502066	0.192259
19	125.293	1.287e-009	0.0042868	0.268151	0.5079	0.219662
20	128.714	2.356e-010	0.00199519	0.225168	0.488178	0.284659
21	135.352	3.879e-011	0.000796653	0.164494	0.41764	0.417068

Example 02

Separation of Paraffins

Sum xD = 1; Iterations = 11

Component	xD	xB
nonane	0.1414	0.0131744
n-decane	0.596271	0.182636
undecane	0.242862	0.234126
n-dodacane	0.0193242	0.211186
n-tridecane	0.000112482	0.206654
n-tetradecane	2.78852e-007	0.152222

Plate number	T °C	Liquid Compositions					
		nonane	n-decane	undecane	dodacane	n-tridecane	n-tetradecane
1	166.386	0.0664768	0.508825	0.371679	0.0524783	0.000538913	2.32932e-006
2	169.841	0.0453891	0.434624	0.4301	0.088473	0.00140436	9.7253e-006
3	172.08	0.0390403	0.386186	0.446406	0.125265	0.00306791	3.48182e-005
4	173.771	0.0365833	0.3557	0.440266	0.161187	0.00614689	0.000116285
5	175.225	0.0352064	0.335219	0.423061	0.194489	0.0116536	0.000370827
6	176.607	0.0341454	0.319658	0.400725	0.223179	0.0211559	0.00113673
7	178.046	0.0331365	0.305942	0.375819	0.244878	0.0368764	0.00334801

8	179.697	0.0320172	0.291854	0.348673	0.256586	0.0614556	0.00941421
9	181.799	0.0306113	0.275255	0.318018	0.254493	0.0967084	0.024914
10	184.708	0.0287144	0.253935	0.28181	0.234632	0.140406	0.0605034
11	188.802	0.0261988	0.226683	0.239276	0.195903	0.181879	0.13006
12	189.152	0.0261444	0.226649	0.239298	0.19593	0.181904	0.130074
13	189.501	0.0260785	0.226622	0.239323	0.195959	0.181928	0.130088
14	189.849	0.0259916	0.226608	0.239353	0.19599	0.181954	0.130103
15	190.198	0.0258671	0.226613	0.239394	0.196025	0.181982	0.130119
16	190.55	0.0256754	0.226651	0.239455	0.196067	0.182015	0.130136
17	190.909	0.0253635	0.22673	0.239564	0.196128	0.182056	0.130158
18	191.285	0.0248356	0.226827	0.239792	0.196238	0.18212	0.130188
19	191.706	0.0239164	0.226733	0.240334	0.196508	0.18226	0.130248
20	192.254	0.0222719	0.225404	0.241652	0.197432	0.18278	0.130461
21	193.293	0.0192133	0.218016	0.243762	0.201067	0.185843	0.132098
22	196.921	0.0131744	0.182636	0.234126	0.211186	0.206654	0.152222

Example 03

Depropanizer

Sum xD = 0.99366; Iterations = 20

Component	xD	xB
methane	0.436826	5.78242e-015
ethane	0.151209	9.03101e-009
propane	0.411962	0.0118563
n-butane	3.14868e-006	0.419958
n-pentane	2.01843e-011	0.271741
n-hexane	3.90269e-016	0.296444

Plate number	T °C	Liquid Compositions					
		methane	ethane	propane	n-butane	n-pentane	n-hexane
1	27.7601	0.0369506	0.0798081	0.883215	2.58773e-005	5.79335e-010	3.73438e-014
2	47.5328	0.0137372	0.0404324	0.945751	7.89281e-005	5.23206e-009	9.91602e-013
3	49.4782	0.0125449	0.0306363	0.956601	0.000217325	4.35799e-008	2.43801e-011
4	49.8101	0.0124619	0.0283654	0.958589	0.000583622	3.58554e-007	5.92303e-010
5	49.919	0.0124496	0.0278333	0.95816	0.00155387	2.93998e-006	1.43368e-008
6	50.0337	0.0124394	0.0276744	0.955745	0.00411664	2.40261e-005	3.45682e-007
7	50.2874	0.0124138	0.0275342	0.94902	0.0108284	0.000194863	8.26162e-006
8	50.9655	0.0123406	0.0272126	0.930717	0.0279885	0.0015482	0.000192778
9	53.089	0.01211	0.0262478	0.877394	0.0685399	0.0115334	0.00417443
10	62.1536	0.0111987	0.0226674	0.69937	0.134392	0.0658976	0.0664739
11	74.0659	0.000797406	0.00723125	0.718066	0.140344	0.0666313	0.0669297
12	76.1219	5.59444e-005	0.00224513	0.711569	0.151317	0.0674086	0.0674045
13	77.8016	3.87744e-006	0.000682051	0.685411	0.177106	0.0687462	0.0680508
14	81.0705	2.62074e-007	0.000198414	0.62431	0.235066	0.0714141	0.0690118
15	87.6466	1.68414e-008	5.2938e-005	0.508724	0.34385	0.0768809	0.0704923
16	98.2741	1.00181e-009	1.23538e-005	0.348578	0.491004	0.0876448	0.0727604
17	110.774	5.48326e-011	2.48755e-006	0.19692	0.617584	0.10842	0.0770732
18	122.273	2.79839e-012	4.41251e-007	0.093891	0.66692	0.148198	0.0909906
19	133.877	1.33661e-013	6.9242e-008	0.0378114	0.605056	0.213131	0.144002
20	150.834	5.78242e-015	9.03101e-009	0.0118563	0.419958	0.271741	0.296444

Example 04

Ethane spliter

Sum xD = 1.0006; Iterations = 20

Component	xD	xB
methane	0.126245	1.85989e-009
ethane	0.873192	0.00690144
propylene	0.000436589	0.248081
propane	0.000126776	0.331073
i-butane	3.20108e-008	0.165578
n-butane	3.08638e-009	0.248367

Plate number	T °C	Liquid Compositions					
		methane	ethane	propylene	propane	i-butane	n-butane
1	2.74452	0.0180278	0.979391	0.00190141	0.000679349	5.12185e-007	7.44004e-008
2	5.8543	0.00794548	0.984287	0.00543238	0.00232972	4.83304e-006	1.03737e-006
3	6.603	0.00700945	0.971624	0.0140335	0.00727586	4.30733e-005	1.37693e-005
4	7.87611	0.00683233	0.937176	0.0340122	0.0214388	0.000366409	0.000174209
5	10.9855	0.00658797	0.856444	0.0747941	0.057393	0.00280908	0.00197204
6	18.129	0.00607987	0.69796	0.135332	0.125972	0.0171576	0.0174989
7	32.8247	0.00519421	0.46653	0.170595	0.190826	0.0684364	0.0984182
8	40.5329	0.000774933	0.387257	0.213519	0.225369	0.0714893	0.101591
9	49.7292	0.000106521	0.275988	0.268496	0.273148	0.0759357	0.106326
10	59.8683	1.34445e-005	0.168098	0.317346	0.322073	0.0809348	0.111535
11	68.4498	1.58374e-006	0.0900521	0.345226	0.360798	0.0866896	0.117233
12	74.6878	1.77664e-007	0.0437178	0.347601	0.384233	0.0965915	0.127856
13	80.189	1.9053e-008	0.0191173	0.319598	0.383114	0.119154	0.159017
14	88.5802	1.85989e-009	0.00690144	0.248081	0.331073	0.165578	0.248367

Example 05

Fractionation-of-Xylenes

Sum xD = 0.989427; Iterations = 20

Component	xD	xB
ethylbenzene	0.0616255	7.47157e-006
p-xylene	0.695841	0.00234939
m-xylene	0.233619	0.00242808
o-xylene	0.00891477	0.995215

Plate number	T °C	Liquid Compositions			
		E.B	p-xylene	m-xylene	o-xylene
1	138.455	0.058015	0.693829	0.237692	0.0104642
2	138.621	0.0548861	0.69165	0.241347	0.0121173
3	138.787	0.0521743	0.689332	0.244614	0.0138798
4	138.951	0.0498237	0.686899	0.24752	0.0157574
5	139.114	0.0477852	0.684367	0.250092	0.0177561
6	139.277	0.0460163	0.68175	0.252351	0.019882
7	139.44	0.0444801	0.679059	0.254319	0.0221415
8	139.602	0.0431442	0.6763	0.256015	0.0245408
9	139.765	0.0419809	0.673478	0.257455	0.0270866
10	139.927	0.0409659	0.670594	0.258655	0.0297854
11	140.089	0.0400783	0.667649	0.259629	0.0326438
12	140.251	0.0392998	0.664643	0.260389	0.0356683
13	140.414	0.0386147	0.661573	0.260946	0.0388655
14	140.577	0.0380094	0.658437	0.261312	0.0422415
15	140.74	0.0374721	0.655231	0.261495	0.0458025
16	140.903	0.0369925	0.65195	0.261503	0.0495544
17	141.067	0.0365619	0.648591	0.261344	0.0535026
18	141.232	0.0361725	0.64515	0.261026	0.0576522
19	141.397	0.0358179	0.641621	0.260554	0.0620078
20	141.563	0.0354923	0.638	0.259934	0.0665733
21	141.73	0.0351908	0.634285	0.259173	0.071352
22	141.897	0.0349092	0.63047	0.258275	0.0763463
23	142.065	0.0346438	0.626554	0.257245	0.0815578
24	142.234	0.0343916	0.622533	0.256088	0.0869873
25	142.404	0.0341499	0.618406	0.25481	0.0926342
26	142.574	0.0339165	0.614171	0.253415	0.0984971
27	142.745	0.0336893	0.60983	0.251908	0.104573
28	142.917	0.033467	0.605381	0.250293	0.110859
29	143.09	0.033248	0.600827	0.248577	0.117348
30	143.264	0.0330314	0.596171	0.246763	0.124034
31	143.438	0.0328162	0.591416	0.244859	0.130909
32	143.613	0.0326019	0.586566	0.242868	0.137964

33	143.788	0.0323878	0.581627	0.240798	0.145187
34	143.964	0.0321736	0.576606	0.238654	0.152567
35	144.141	0.0319591	0.571509	0.236443	0.160089
36	144.318	0.0317441	0.566346	0.234172	0.167739
37	144.495	0.0315288	0.561125	0.231846	0.1755
38	144.672	0.031313	0.555856	0.229474	0.183357
39	144.85	0.0310971	0.55055	0.227063	0.19129
40	145.027	0.0308813	0.545217	0.224619	0.199282
41	145.205	0.0306657	0.539871	0.222151	0.207313
42	145.382	0.0304508	0.534521	0.219665	0.215363
43	145.559	0.0302369	0.529181	0.21717	0.223412
44	145.736	0.0300243	0.523863	0.214671	0.231441
45	145.912	0.0298136	0.518579	0.212177	0.23943
46	146.088	0.0296051	0.51334	0.209695	0.24736
47	146.304	0.0274028	0.502357	0.209055	0.261185
48	146.527	0.0253051	0.490438	0.207912	0.276344
49	146.758	0.0233089	0.477566	0.206234	0.292891
50	146.997	0.0214115	0.463737	0.203991	0.310861
51	147.244	0.0196107	0.448959	0.201159	0.330271
52	147.498	0.0179049	0.433261	0.197722	0.351112
53	147.761	0.0162928	0.416688	0.193674	0.373346
54	148.031	0.0147733	0.399306	0.189016	0.396905
55	148.307	0.0133458	0.381204	0.183763	0.421687
56	148.591	0.0120095	0.362488	0.177944	0.447559
57	148.879	0.0107636	0.343286	0.171596	0.474355
58	149.172	0.00960727	0.323739	0.164773	0.50188
59	149.468	0.00853917	0.304003	0.157538	0.52992
60	149.766	0.00755765	0.28424	0.149963	0.558239
61	150.063	0.00666056	0.264615	0.142128	0.586597
62	150.36	0.00584522	0.245288	0.134116	0.61475
63	150.654	0.00510839	0.226413	0.126014	0.642465
64	150.945	0.00444635	0.208127	0.117906	0.66952
65	151.23	0.00385492	0.190553	0.109872	0.69572
66	151.509	0.00332955	0.173792	0.101985	0.720894
67	151.781	0.00286545	0.157923	0.0943114	0.7449
68	152.045	0.00245764	0.143003	0.0869065	0.767632
69	152.301	0.00210112	0.129069	0.0798159	0.789014
70	152.548	0.00179096	0.116135	0.0730748	0.808999
71	152.786	0.00152234	0.1042	0.0667084	0.82757
72	153.016	0.0012907	0.0932436	0.0607322	0.844734
73	153.236	0.00109173	0.0832364	0.0551537	0.860518
74	153.449	0.000921447	0.0741372	0.0499728	0.874969
75	153.653	0.000776201	0.0658976	0.0451834	0.888143
76	153.849	0.000652687	0.0584645	0.0407744	0.900108
77	154.038	0.000547945	0.0517817	0.036731	0.910939
78	154.221	0.000459344	0.0457917	0.0330354	0.920714

79	154.396	0.000384565	0.0404375	0.029668	0.92951
80	154.567	0.00032158	0.0356635	0.026608	0.937407
81	154.731	0.000268624	0.031416	0.0238341	0.944481
82	154.891	0.000224172	0.0276446	0.021325	0.950806
83	155.046	0.000186912	0.0243015	0.0190598	0.956452
84	155.197	0.000155719	0.0213429	0.0170183	0.961483
85	155.344	0.000129636	0.018728	0.0151813	0.965961
86	155.488	0.000107846	0.0164197	0.0135303	0.969942
87	155.629	8.96586e-005	0.0143843	0.0120484	0.973478
88	155.767	7.449e-005	0.0125911	0.0107196	0.976615
89	155.902	6.18473e-005	0.0110126	0.00952923	0.979396
90	156.036	5.13159e-005	0.00962419	0.00846366	0.981861
91	156.167	4.25478e-005	0.00840367	0.00751051	0.984043
92	156.296	3.52508e-005	0.00733135	0.00665844	0.985975
93	156.424	2.91803e-005	0.00638967	0.00589714	0.987684
94	156.55	2.41318e-005	0.00556307	0.00521727	0.989196
95	156.675	1.99344e-005	0.00483774	0.00461037	0.990532
96	156.799	1.64454e-005	0.00420147	0.00406879	0.991713
97	156.921	1.35458e-005	0.00364346	0.00358566	0.992757
98	157.043	1.11364e-005	0.00315421	0.00315477	0.99368
99	157.163	9.13459e-006	0.00272531	0.00277058	0.994495
100	157.283	7.47157e-006	0.00234939	0.00242808	0.995215

Example 06

Separation of Ethylbenzene-Styrene

Sum Xd = 0.999906; Iterations = 20

Component	xD	xB
toluene	0.0220021	1.96824e-017
ethylbenzene	0.962522	0.0775609
styrene	0.0154664	0.914449
isopropylbenzene	9.39492e-006	0.00798986

Plate number	T °C	Liquid Compositions			
		toluene	E.B	styrene	i-propylebenzene
1	57.5126	0.00874479	0.969027	0.0222119	1.58625e-005
2	59.0355	0.0041225	0.965544	0.0303084	2.50885e-005
3	60.4067	0.00252107	0.957404	0.0400371	3.82182e-005
4	61.7011	0.00196787	0.946307	0.051668	5.6795e-005
5	62.949	0.00177733	0.932684	0.0654559	8.28746e-005
6	64.165	0.00171151	0.916541	0.0816286	0.000119155
7	65.3572	0.00168764	0.897777	0.100366	0.000169115
8	66.5313	0.0016769	0.87631	0.121776	0.000237142
9	67.6909	0.00166927	0.852141	0.145861	0.000328649

10	68.8385	0.00166134	0.825391	0.172498	0.000450142
11.	69.9751	0.00165205	0.796323	0.201416	0.00060924
12	71.1002	0.00164128	0.76535	0.232194	0.000814631
13	72.2122	0.00162923	0.733017	0.264277	0.00107599
14	73.3081	0.0016163	0.699971	0.297009	0.00140383
15	74.3843	0.00160295	0.666909	0.329679	0.00180948
16	75.437	0.00158964	0.634522	0.361584	0.00230494
17	76.2658	0.00068572	0.633873	0.363129	0.00231198
18	77.055	0.000296476	0.632805	0.36458	0.00231835
19	77.8173	0.000128504	0.631519	0.366028	0.00232449
20	78.559	5.58388e-005	0.630087	0.367527	0.00233062
21	79.2832	2.43236e-005	0.628525	0.369114	0.00233689
22	79.992	1.06207e-005	0.626821	0.370825	0.00234339
23	80.6867	4.64796e-006	0.624948	0.372698	0.00235023
24	81.3687	2.03848e-006	0.622866	0.374775	0.00235752
25	82.0391	8.95826e-007	0.620526	0.377108	0.00236539
26	82.6989	3.94414e-007	0.617867	0.379759	0.00237399
27	83.3494	1.73949e-007	0.614815	0.382801	0.00238351
28	83.9918	7.68335e-008	0.611284	0.386322	0.00239418
29	84.6275	3.3982e-008	0.607169	0.390425	0.00240626
30	85.258	1.50458e-008	0.602348	0.395232	0.00242007
31	85.8848	6.66696e-009	0.59668	0.400884	0.00243598
32	86.5096	2.95567e-009	0.590003	0.407543	0.00245443
33	87.1345	1.31051e-009	0.582134	0.41539	0.00247594
34	87.7615	5.80912e-010	0.572873	0.424626	0.00250111
35	88.3928	2.57312e-010	0.562003	0.435466	0.00253063
36	89.0306	1.13832e-010	0.549302	0.448132	0.00256529
37	89.6774	5.02664e-011	0.534552	0.462842	0.00260602
38	90.3351	2.21423e-011	0.517554	0.479792	0.00265384
39	91.0057	9.72321e-012	0.49815	0.49914	0.00270998
40	91.6907	4.25338e-012	0.476246	0.520978	0.00277586
41	92.3907	1.85221e-012	0.451838	0.545309	0.00285318
42	93.1056	8.02382e-013	0.425031	0.572025	0.00294406
43	93.8341	3.45569e-013	0.396058	0.600891	0.00305122
44	94.5739	1.47882e-013	0.365284	0.631538	0.0031782
45	95.3213	6.2856e-014	0.333192	0.663478	0.00332973
46	96.0719	2.65281e-014	0.300361	0.696127	0.0035122
47	96.8207	1.11159e-014	0.26742	0.728846	0.00373419
48	97.5621	4.62451e-015	0.235005	0.760988	0.0040072
49	98.2909	1.91033e-015	0.203707	0.791946	0.0043465
50	99.0026	7.8355e-016	0.174033	0.821195	0.00477215
51	99.6934	3.18958e-016	0.146374	0.848316	0.00531034
52	100.361	1.28618e-016	0.120998	0.873007	0.00599492
53	101.003	5.10925e-017	0.0980493	0.895081	0.00686949
54	101.62	1.96824e-017	0.0775609	0.914449	0.00798986

Example 07

Seperation-of-Toluene_Ethylbenzene

Sum xD = 0.999935; Iterations = 20

Component	xD	xB
benzene	0.364718	0.00174756
toluene	0.485705	0.0496709
ethylbenzene	0.126924	0.452146
styrene	0.0226531	0.496435

Plate number	T °C	Liquid Compositions			
		benzene	toluene	E.B	styrene
1	63.8331	0.130412	0.481425	0.31014	0.078023
2	73.5783	0.0458591	0.338554	0.459435	0.156152
3	79.833	0.0232007	0.209843	0.527866	0.239091
4	83.6244	0.0173611	0.134009	0.531071	0.317559
5	85.986	0.0155663	0.096278	0.498208	0.389947
6	87.606	0.0148311	0.0785797	0.449808	0.456781
7	88.7363	0.0101524	0.0774429	0.453029	0.459375
8	89.8247	0.006537	0.0738976	0.456447	0.463119
9	90.9939	0.00379312	0.0658862	0.45898	0.47134
10	92.5062	0.00174756	0.0496709	0.452146	0.496435

Example 08

Biphenyl-separation

Sum xD = 1.00054; Iterations = 20

Component	xD	xB
benzene	0.950021	4.12577e-006
toluene	0.0499787	0.00406819
diphenyl	4.38392e-007	0.995928

Plate number	T °C	Liquid Compositions		
		benzene	toluene	diphenyl
1	95.8182	0.885365	0.114628	7.30288e-006
2	97.4694	0.819949	0.179989	6.12104e-005
3	99.0779	0.759331	0.240206	0.00046363
4	100.597	0.70621	0.29046	0.0033307
5	102.428	0.653748	0.323658	0.0225948
6	108.565	0.450295	0.526601	0.0231031
7	115.204	0.263297	0.713047	0.0236553
8	120.477	0.1359	0.839394	0.024706
9	123.918	0.0648751	0.905078	0.0300465
10	126.837	0.0290369	0.907598	0.0633651

11	134.277	0.0110264	0.756724	0.23225
12	157.428	0.00259945	0.369885	0.627515
13	187.417	0.000357774	0.0990387	0.900604
14	201.256	3.947e-005	0.0207008	0.97926
15	204.812	4.12577e-006	0.00406819	0.995928

Example 9

Phenol-Cresol-separation

Sum xD = 1.00038; Iterations = 20

Component	xD	xB
phenol	0.955407	0.0502928
o-cresol	0.0445561	0.2022
m-cresol	3.70723e-005	0.448497
2,3 xylenol	1.17629e-008	0.29901

Plate number	T °C	Liquid Compositions			
		phenol	o-cresol	m-cresol	2,3 xylenol
1	131.533	0.943461	0.0564682	7.11842e-005	3.49771e-008
2	132.323	0.929906	0.0699637	0.000130142	9.71648e-008
3	133.109	0.91462	0.0851488	0.000231456	2.62671e-007
4	133.895	0.897491	0.102104	0.000404483	7.00108e-007
5	134.68	0.878431	0.120869	0.000698004	1.84773e-006
6	135.469	0.85737	0.141433	0.00119231	4.8347e-006
7	136.261	0.834261	0.163709	0.00201812	1.25426e-005
8	137.062	0.809064	0.187518	0.00338565	3.22486e-005
9	137.874	0.781734	0.212556	0.00562803	8.21171e-005
10	138.704	0.75218	0.23835	0.00926366	0.000206886
11	139.562	0.720209	0.264195	0.0150803	0.000515
12	140.465	0.685447	0.289054	0.0242343	0.00126416
13	141.442	0.647218	0.311396	0.0383347	0.00305068
14	142.539	0.604412	0.328969	0.0594149	0.00720316
15	143.836	0.555386	0.338533	0.0895659	0.0165149
16	145.455	0.498111	0.335754	0.129806	0.0363293
17	147.564	0.431031	0.315875	0.177768	0.0753255
18	148.541	0.394436	0.339023	0.189791	0.0767499
19	149.61	0.3541	0.360212	0.206811	0.0788764
20	150.8	0.310404	0.376758	0.230534	0.0823042
21	152.151	0.264059	0.385177	0.262544	0.0882201
22	153.714	0.216225	0.38145	0.303432	0.0988929
23	155.55	0.168599	0.361768	0.351277	0.118356
24	157.726	0.123409	0.32387	0.399768	0.152953
25	160.299	0.0831984	0.268801	0.437181	0.21082
26	163.281	0.0502928	0.2022	0.448497	0.29901

TGXBPTH

Example 01

Depropanizer

Iterations = 7; Theta = 1.00013

Component	xD	xB
ethane	0.0145259	7.58553e-011
propane	0.983173	0.00205895
i-butane	0.00204627	0.166454
n-butane	0.000255183	0.41617
n-pentane	6.36993e-009	0.415317

Plate	T °C	Liquid Compositions				
number		ethane	propane	i-butane	n-butane	n-pentane
1	62.3021	0.00430204	0.989914	0.00495506	0.000829216	6.02746e-008
2	62.7299	0.00236602	0.986301	0.009339	0.00199328	3.79473e-007
3	63.0747	0.00199472	0.977769	0.0158976	0.00433616	2.25247e-006
4	63.5641	0.00191239	0.963551	0.0255421	0.00898139	1.30863e-005
5	64.3428	0.00187614	0.940786	0.039302	0.0179615	7.43088e-005
6	65.5936	0.0018361	0.905186	0.0579541	0.0346162	0.000407538
7	67.5796	0.00177761	0.85149	0.0811244	0.0634918	0.00211663
8	70.7078	0.00169069	0.774247	0.105676	0.108284	0.0101027
9	75.787	0.00156209	0.667802	0.12353	0.16492	0.0421857
10	84.5715	0.001371	0.527826	0.121152	0.208472	0.141178
11	87.6327	0.000404115	0.47529	0.148323	0.231612	0.144371
12	92.2301	0.0001123	0.396963	0.186852	0.266925	0.149148
13	98.37	2.8996e-005	0.300721	0.231606	0.312467	0.155177
14	105.172	6.90551e-006	0.205237	0.272227	0.361089	0.16144

15	111.352	1.5332e-006	0.127781	0.299889	0.405285	0.167043
16	116.122	3.23019e-007	0.0742	0.311897	0.441792	0.172111
17	119.497	6.56331e-008	0.0409733	0.309833	0.470876	0.178318
18	122.012	1.2984e-008	0.0217187	0.295664	0.492571	0.190047
19	124.509	2.49947e-009	0.0109862	0.269185	0.502185	0.217643
20	128.262	4.59701e-010	0.00514146	0.227176	0.484992	0.282691
21	135.091	7.58553e-011	0.00205895	0.166454	0.41617	0.415317

Example 02

Separation of Paraffins

Iterations = 10; Theta = 0.999992

Component	xD	xB
nonane	0.14143	0.0131745
n-decane	0.596272	0.182637
undecane	0.242861	0.234127
n-dodacane	0.0193242	0.211186
n-tridecane	0.000112482	0.206654
n-tetradecane	2.78853e-007	0.152222

Plate number	T °C	Liquid Compositions					
		nonane	n-decane	undecane	n-dodacane	n-tridecane	n-tetradecane
1	166.386	0.0664768	0.508825	0.371679	0.0524781	0.000538913	2.32932e-006
2	169.841	0.0453892	0.434625	0.430099	0.0884727	0.00140436	9.72529e-006
3	172.08	0.0390404	0.386187	0.446405	0.125265	0.0030679	3.48181e-005
4	173.772	0.0365834	0.355701	0.440266	0.161186	0.00614688	0.000116284
5	175.225	0.0352066	0.33522	0.423061	0.194488	0.0116536	0.000370824
6	176.607	0.0341456	0.319659	0.400725	0.223178	0.0211558	0.00113673
7	178.046	0.0331365	0.305943	0.37582	0.244877	0.0368762	0.00334799
8	179.696	0.0320171	0.291854	0.348674	0.256585	0.0614554	0.00941417

9	181.799	0.0306113	0.275255	0.318019	0.254492	0.0967082	0.024914
10	184.708	0.0287144	0.253935	0.28181	0.234632	0.140406	0.0605033
11	188.802	0.0261987	0.226683	0.239276	0.195903	0.181879	0.13006
12	189.152	0.0261443	0.226649	0.239298	0.195931	0.181904	0.130074
13	189.501	0.0260784	0.226622	0.239323	0.195959	0.181929	0.130089
14	189.849	0.0259915	0.226608	0.239353	0.19599	0.181954	0.130103
15	190.198	0.025867	0.226613	0.239394	0.196025	0.181983	0.130119
16	190.549	0.0256754	0.226651	0.239455	0.196068	0.182015	0.130137
17	190.908	0.0253634	0.22673	0.239564	0.196129	0.182056	0.130158
18	191.285	0.0248356	0.226826	0.239792	0.196238	0.18212	0.130188
19	191.706	0.0239163	0.226732	0.240334	0.196508	0.18226	0.130248
20	192.254	0.0222719	0.225403	0.241652	0.197432	0.18278	0.130461
21	193.293	0.0192133	0.218016	0.243762	0.201067	0.185843	0.132098
22	196.921	0.0131745	0.182637	0.234127	0.211186	0.206654	0.152222

Example 03

Depropanizer

Iterations = 11; Theta = 1.00021

Component	xD	xB
methane	0.434057	2.92547e-015
ethane	0.15025	2.66614e-009
propane	0.415689	0.00249979
n-butane	3.60639e-006	0.423934
n-pentane	2.15972e-011	0.274314
n-hexane	4.20251e-016	0.299252

Plate number	T °C	Liquid Compositions					
		methane	ethane	propane	n-butane	n-pentane	n-hexane
1	28.0596	0.0366083	0.0788552	0.884507	2.93619e-005	6.12896e-010	3.96813e-014
2	47.654	0.0136344	0.0399996	0.946277	8.93151e-005	5.51395e-009	1.04876e-012
3	49.5733	0.0124578	0.0303613	0.956936	0.000245343	4.57823e-008	2.56896e-011
4	49.9022	0.0123758	0.0281307	0.958836	0.000657254	3.75516e-007	6.21887e-010
5	50.0144	0.0123631	0.0276069	0.958281	0.00174539	3.06931e-006	1.49976e-008
6	50.139	0.0123518	0.0274456	0.955567	0.0046107	2.49961e-005	3.60162e-007
7	50.4194	0.0123233	0.0272941	0.948088	0.0120847	0.000201861	8.56495e-006
8	51.1646	0.0122432	0.026944	0.92795	0.0310707	0.00159369	0.000198394
9	53.445	0.0119981	0.0259196	0.870706	0.0753921	0.0117427	0.0042417
10	62.7514	0.0110743	0.0222993	0.688735	0.145719	0.0659531	0.0662187
11	75.6021	0.000776075	0.00693576	0.687003	0.171373	0.0672297	0.0666828
12	80.0361	5.25987e-005	0.00203184	0.63388	0.226964	0.0695789	0.0674926
13	86.5612	3.3986e-006	0.000546491	0.523342	0.332872	0.0741804	0.0690558
14	96.8285	2.04381e-007	0.000129309	0.365785	0.481371	0.0813382	0.0713759
15	108.705	1.13663e-008	2.66189e-005	0.213333	0.622495	0.0902922	0.0738532
16	118.552	5.94636e-010	4.91501e-006	0.107968	0.713817	0.10194	0.0762702
17	125.267	2.9894e-011	8.45387e-007	0.049736	0.748262	0.121532	0.0804693
18	130.583	1.45764e-012	1.37648e-007	0.0212347	0.725214	0.158807	0.0947439
19	138.016	6.81642e-014	2.07524e-008	0.0081258	0.623894	0.219841	0.148138
20	152.589	2.92547e-015	2.66614e-009	0.00249979	0.423934	0.274314	0.299252

Example 04

Ethane-splitter

Iterations = 8 Theta = 0.999986

Component	xD	xB
methane	0.12987	3.29163e-009
ethane	0.86987	0.0245528
propylene	0.000198494	0.243778
propane	6.13417e-005	0.325165
i-butane	1.62413e-008	0.162602
n-butane	1.53337e-009	0.243902

Plate number	T °C	Liquid Compositions					
		methane	ethane	propylene	propane	i-butane	n-butane
1	2.53948	0.018591	0.980208	0.000869703	0.000330755	2.61751e-007	3.72512e-008
2	5.75005	0.00784037	0.988438	0.00255128	0.00116706	2.55868e-006	5.38841e-007
3	6.29395	0.00682731	0.982494	0.00685084	0.00379603	2.38676e-005	7.49424e-006
4	7.00648	0.00668043	0.963537	0.0175909	0.0118731	0.000216808	0.00010149
5	8.89613	0.0065199	0.912881	0.0424731	0.0349904	0.00185001	0.00128565
6	14.0939	0.00612478	0.788982	0.0888121	0.0890995	0.0133599	0.0136213
7	27.8299	0.0052458	0.547526	0.131255	0.158906	0.0640258	0.0930413
8	31.1347	0.000845581	0.526903	0.14438	0.169093	0.0648768	0.093901
9	34.8	0.000131405	0.474323	0.171708	0.191435	0.0666876	0.095716
10	41.4605	1.91464e-005	0.379458	0.218138	0.232954	0.0702257	0.0992061
11	51.551	.543e-006	0.25581	0.272849	0.289834	0.0763742	0.10513
12	62.9031	3.06302e-007	0.143163	0.309559	0.342476	0.0878246	0.116978
13	73.6037	3.37474e-008	0.0668018	0.305093	0.365003	0.112831	0.150272
14	85.6621	3.29161e-009	0.0245527	0.243778	0.325165	0.162602	0.243903

Example 05

Fractionation-of-Xylenes

Iterations = 10; Theta = 0.999849

Component	xD	xB
ethylbenzene	0.0609748	3.63296e-006
p-xylene	0.688784	0.00109442
m-xylene	0.231465	0.0011035
o-xylene	0.0187763	0.997798

Plate number	T °C	Liquid Compositions			
		E.B	p-xylene	m-xylene	o-xylene
1	138.52	0.0573041	0.685605	0.23509	0.0220006
2	138.696	0.0541151	0.682195	0.238262	0.0254277
3	138.872	0.0513436	0.678581	0.24101	0.0290656
4	139.047	0.0489333	0.674786	0.243359	0.0329217
5	139.222	0.0468353	0.670826	0.245335	0.0370037
6	139.397	0.0450067	0.666716	0.246959	0.0413183
7	139.573	0.0434103	0.662465	0.248252	0.0458721
8	139.748	0.0420138	0.658082	0.249234	0.050671
9	139.925	0.040789	0.653571	0.24992	0.05572
10	140.101	0.0397116	0.648937	0.250328	0.0610233
11	140.278	0.0387605	0.644183	0.250473	0.066584
12	140.456	0.0379173	0.639311	0.250368	0.0724042
13	140.635	0.0371663	0.634323	0.250026	0.0784845
14	140.814	0.0364938	0.629221	0.249461	0.0848242
15	140.995	0.035888	0.624007	0.248684	0.091421
16	141.176	0.0353389	0.618683	0.247707	0.0982709
17	141.358	0.0348377	0.613252	0.246542	0.105368
18	141.54	0.034377	0.607718	0.245199	0.112705
19	141.724	0.0339505	0.602086	0.243691	0.120273
20	141.907	0.0335528	0.59636	0.242027	0.12806
21	142.092	0.0331793	0.590548	0.240219	0.136054
22	142.278	0.0328261	0.584658	0.238278	0.144238
23	142.464	0.0324901	0.578697	0.236217	0.152597
24	142.651	0.0321686	0.572676	0.234045	0.161111
25	142.838	0.0318594	0.566605	0.231774	0.169762
26	143.025	0.0315608	0.560496	0.229417	0.178526
27	143.212	0.0312714	0.554362	0.226984	0.187383
28	143.4	0.03099	0.548215	0.224487	0.196308
29	143.587	0.0307159	0.54207	0.221937	0.205277
30	143.774	0.0304484	0.53594	0.219347	0.214264

31	143.961	0.0301871	0.52984	0.216727	0.223246
32	144.147	0.0299317	0.523783	0.214087	0.232198
33	144.333	0.0296821	0.517785	0.21144	0.241094
34	144.518	0.0294382	0.511858	0.208793	0.249911
35	144.702	0.0292	0.506016	0.206159	0.258626
36	144.885	0.0289677	0.500272	0.203544	0.267216
37	145.067	0.0287413	0.494637	0.200959	0.275662
38	145.247	0.028521	0.489124	0.198411	0.283944
39	145.427	0.028307	0.483742	0.195907	0.292045
40	145.604	0.0280994	0.4785	0.193453	0.299948
41	145.781	0.0278984	0.473406	0.191057	0.307639
42	145.955	0.0277041	0.468468	0.188722	0.315107
43	146.129	0.0275167	0.463691	0.186453	0.32234
44	146.3	0.0273361	0.459079	0.184254	0.329331
45	146.47	0.0271627	0.454637	0.182127	0.336073
46	146.638	0.0269962	0.450367	0.180076	0.34256
47	146.906	0.0245873	0.433622	0.176622	0.365169
48	147.182	0.0223118	0.415953	0.172583	0.389152
49	147.466	0.0201696	0.397455	0.167973	0.414402
50	147.756	0.0181604	0.378243	0.162816	0.44078
51	148.051	0.0162841	0.358454	0.157149	0.468113
52	148.351	0.0145399	0.338241	0.151019	0.4962
53	148.653	0.0129267	0.317774	0.144486	0.524813
54	148.958	0.0114426	0.29723	0.137618	0.55371
55	149.262	0.0100849	0.276786	0.130491	0.582638
56	149.566	0.00885007	0.256621	0.123184	0.611345
57	149.866	0.0077335	0.2369	0.115779	0.639588
58	150.162	0.00672988	0.217776	0.108355	0.667139
59	150.453	0.0058331	0.199382	0.10099	0.693795
60	150.738	0.00503643	0.181829	0.0937524	0.719382
61	151.015	0.0043327	0.165205	0.0867052	0.743757
62	151.283	0.00371444	0.149573	0.0799014	0.766812
63	151.544	0.0031741	0.134972	0.0733843	0.788469
64	151.795	0.00270418	0.121422	0.0671875	0.808687
65	152.037	0.00229739	0.108919	0.0613348	0.827449
66	152.269	0.00194677	0.0974461	0.0558412	0.844766
67	152.493	0.00164577	0.0869703	0.050714	0.86067
68	152.708	0.00138832	0.0774487	0.0459532	0.87521
69	152.915	0.00116886	0.0688306	0.0415533	0.888447
70	153.114	0.000982353	0.0610596	0.0375042	0.900454
71	153.305	0.000824299	0.0540763	0.0337919	0.911308
72	153.49	0.00069069	0.0478202	0.0304001	0.921089

73	153.667	0.000578001	0.042231	0.0273106	0.92988
74	153.839	0.000483148	0.0372499	0.0245042	0.937763
75	154.006	0.000403453	0.0328206	0.021961	0.944815
76	154.167	0.0003366	0.0288895	0.0196615	0.951112
77	154.324	0.000280599	0.0254068	0.0175862	0.956726
78	154.476	0.000233749	0.022326	0.0157165	0.961724
79	154.625	0.000194598	0.0196044	0.0140346	0.966166
80	154.771	0.000161912	0.0172031	0.0125236	0.970111
81	154.913	0.000134647	0.0150866	0.0111677	0.973611
82	155.053	0.000111921	0.0132229	0.00995233	0.976713
83	155.19	9.29915e-5	0.011583	0.00886382	0.97946
84	155.324	7.72322e-5	0.0101412	0.00788974	0.981892
85	155.457	6.41191e-5	0.00887427	0.00701867	0.984043
86	155.588	5.32123e-5	0.00776162	0.00624019	0.985945
87	155.717	4.4144e-5	0.00678493	0.00554483	0.987626
88	155.845	3.66065e-5	0.00592794	0.004924	0.989111
89	155.971	3.03432e-5	0.00517622	0.00436994	0.990423
90	156.096	2.51397e-5	0.00451705	0.00387563	0.991582
91	156.22	2.08176e-5	0.00393918	0.00343478	0.992605
92	156.343	1.7228e-5	0.0034327	0.00304169	0.993508
93	156.465	1.42473e-5	0.00298886	0.00269128	0.994306
94	156.586	1.17723e-5	0.00259998	0.00237896	0.995009
95	156.707	9.71739e-6	0.0022593	0.00210065	0.99563
96	156.826	8.01139e-6	0.00196087	0.00185267	0.996178
97	156.945	6.5951e-6	0.00169948	0.00163175	0.996662
98	157.064	5.41934e-6	0.00147053	0.00143495	0.997089
99	157.182	4.44327e-6	0.00127002	0.00125964	0.997466
100	157.299	3.63296e-6	0.00109442	0.0011035	0.997798

Example 06

Separation of Ethylbenzene-Styrene

Iterations = 11; Theta = 0.999965

Component	xD	xB
benzene	0.0220001	1.96535e-017
ethylbenzene	0.962524	0.0774779
styrene	0.0154662	0.914532
i-propylbenzene	9.39465e-006	0.00799058

Plate number	T °C	Liquid Compositions			
		toluene	E.B	styrene	i-propylebenzene
1	330.663	0.00874399	0.969029	0.0222115	1.5862e-005
2	332.185	0.00412212	0.965545	0.0303078	2.50877e-005
3	333.557	0.00252084	0.957405	0.0400364	3.8217e-005
4	334.851	0.00196769	0.946308	0.0516671	5.67932e-005
5	336.099	0.00177718	0.932685	0.0654547	8.2872e-005
6	337.315	0.00171136	0.916542	0.0816271	0.000119151
7	338.507	0.00168749	0.897779	0.100365	0.000169109
8	339.681	0.00167676	0.876313	0.121773	0.000237134
9	340.841	0.00166913	0.852144	0.145858	0.000328638
10	341.988	0.0016612	0.825394	0.172494	0.000450127
11	343.125	0.00165192	0.796327	0.201411	0.000609219
12	344.25	0.00164115	0.765355	0.232189	0.000814603
13	345.362	0.0016291	0.733023	0.264272	0.00107595
14	346.458	0.00161616	0.699977	0.297003	0.00140379
15	347.534	0.00160281	0.666915	0.329673	0.00180942
16	348.587	0.00158951	0.634528	0.361577	0.00230487
17	349.416	0.000685655	0.633881	0.363121	0.00231188
18	350.205	0.000296444	0.632815	0.36457	0.00231824
19	350.967	0.000128488	0.631529	0.366018	0.00232436
20	351.709	5.58308e-005	0.630096	0.367518	0.00233049
21	352.433	2.43197e-005	0.628532	0.369107	0.00233676
22	353.142	1.06187e-005	0.626825	0.370821	0.00234327
23	353.837	4.64701e-006	0.624948	0.372697	0.00235012
24	354.519	2.03801e-006	0.622862	0.374779	0.00235742
25	355.189	8.95602e-007	0.620516	0.377117	0.0023653
26	355.849	3.94305e-007	0.61785	0.379775	0.00237393
27	356.5	1.73896e-007	0.614791	0.382825	0.00238349
28	357.142	7.68079e-008	0.61125	0.386356	0.0023942
29	357.778	3.39696e-008	0.607124	0.39047	0.00240632
30	358.408	1.50398e-008	0.602291	0.395289	0.00242018

31	359.035	6.66407e-009	0.596609	0.400955	0.00243616
32	359.661	2.95428e-009	0.589917	0.407628	0.00245468
33	360.286	1.30985e-009	0.582033	0.415491	0.00247626
34	360.913	5.80593e-010	0.572755	0.424744	0.0025015
35	361.544	2.5716e-010	0.561867	0.435602	0.0025311
36	362.182	1.1376e-010	0.549148	0.448286	0.00256585
37	362.829	5.02321e-011	0.53438	0.463013	0.00260666
38	363.487	2.21261e-011	0.517365	0.47998	0.00265456
39	364.158	9.71562e-012	0.497946	0.499344	0.00271077
40	364.843	4.24984e-012	0.476028	0.521195	0.00277671
41	365.543	1.85057e-012	0.451609	0.545537	0.00285408
42	366.258	8.01627e-013	0.424793	0.572262	0.00294501
43	366.986	3.45225e-013	0.395816	0.601132	0.0030522
44	367.726	1.47727e-013	0.365041	0.63178	0.0031792
45	368.473	6.27864e-014	0.332953	0.663717	0.00333075
46	369.224	2.64973e-014	0.300129	0.696358	0.00351322
47	369.973	1.11024e-014	0.2672	0.729064	0.0037352
48	370.714	4.61868e-015	0.234801	0.761191	0.00400819
49	371.443	1.90783e-015	0.203522	0.792131	0.00434746
50	372.154	7.82494e-016	0.173867	0.82136	0.00477308
51	372.845	3.18516e-016	0.146229	0.84846	0.00531122
52	373.512	1.28436e-016	0.120875	0.873129	0.00599576
53	374.154	5.10186e-017	0.0979467	0.895183	0.00687028
54	374.771	1.96535e-017	0.0774779	0.914532	0.00799058

Example 07

Seperation-of-Toluene_Ethyl-benzene

Iterations = 13; Theta = 1

Component	xD	xB
benzene	0.364695	0.00174751
toluene	0.485694	0.0496699
ethylbenzene	0.126952	0.452146
styrene	0.0226593	0.496437

Plate number	T °C	Liquid Compositions			
		Benzene	Toluene	EB	Styrene
1	63.8346	0.130396	0.481382	0.310184	0.0780379
2	73.5797	0.0458528	0.338508	0.459469	0.15617
3	79.834	0.0231986	0.209813	0.527882	0.239106
4	83.6247	0.0173605	0.133995	0.531075	0.31757
5	85.9864	0.015566	0.0962726	0.498208	0.389953
6	87.6063	0.014831	0.0785786	0.449808	0.456782
7	88.7365	0.0101522	0.0774417	0.453029	0.459377
8	89.825	0.00653687	0.0738964	0.456447	0.46312
9	90.994	0.00379303	0.065885	0.45898	0.471342
10	92.5066	0.00174751	0.0496699	0.452146	0.496437

Example 08

Biphenyl-separation

Iterations = 6; Theta = 1.0002

Component	xD	xB
benzene	0.950531	1.46351e-005
toluene	0.0494683	0.0165841
biphenyl	4.35477e-007	0.983401

Plate number	T °C	Liquid Compositions		
		benzene	toluene	diphenyl
1	95.7934	0.886448	0.113544	7.26038e-006
2	97.4327	0.821491	0.178449	6.09263e-005
3	99.0326	0.761146	0.238392	0.000462166
4	100.548	0.708111	0.288564	0.00332559
5	102.379	0.65556	0.321844	0.0225965
6	108.495	0.45248	0.524419	0.0231016
7	115.134	0.265106	0.71131	0.0235835
8	120.407	0.137103	0.838851	0.0240465
9	123.729	0.0657595	0.908989	0.0252515
10	125.748	0.0301915	0.937616	0.0321927
11	128.161	0.0131569	0.911942	0.074901
12	136.718	0.00475166	0.718575	0.276673
13	162.086	0.00102704	0.318738	0.680235
14	190.526	0.000134585	0.0807476	0.919118
15	202.252	1.46351e-005	0.0165841	0.983401

Example 09.

Phenol-Cresol-separation

Iterations = 7; Theta = 1.00006

Component	xD	xB
phenol	0.955516	0.0504098
o-cresol	0.0444468	0.202224
m-cresol	3.69914e-005	0.448412
2,3 xylenol	1.17394e-008	0.298954

Plate number	T °C	Liquid Compositions			
		phenol	o-cresol	m-cresol	2,3 xylenol
1	131.532	0.943597	0.0563315	7.10311e-005	3.49085e-008
2	132.322	0.930073	0.0697968	0.000129867	9.69781e-008
3	133.108	0.91482	0.0849492	0.000230978	2.6218e-007
4	133.893	0.897726	0.101869	0.00040367	6.98841e-007
5	134.679	0.878703	0.120599	0.000696648	1.84452e-006
6	135.467	0.85768	0.141126	0.00119009	4.8267e-006
7	136.259	0.834607	0.163366	0.00201454	1.2523e-005
8	137.059	0.809447	0.187141	0.00337999	3.22018e-005
9	137.871	0.78215	0.212149	0.00561925	8.20075e-005
10	138.701	0.752625	0.237918	0.00925036	0.000206636
11	139.559	0.720678	0.263747	0.0150606	0.000514452
12	140.462	0.685931	0.2886	0.0242063	0.001263
13	141.438	0.647709	0.310947	0.0382963	0.00304839
14	142.536	0.604897	0.328539	0.0593649	0.00719895
15	143.833	0.55585	0.338137	0.0895054	0.0165081
16	145.452	0.498534	0.335407	0.129739	0.0363205
17	147.561	0.43139	0.315587	0.177704	0.0753192
18	148.537	0.394823	0.338727	0.189708	0.0767414
19	149.606	0.354507	0.359924	0.206705	0.0788645
20	150.795	0.310816	0.376495	0.230402	0.0822872
21	152.146	0.26446	0.384957	0.262387	0.088196
22	153.708	0.216595	0.381289	0.303256	0.0988592
23	155.544	0.168919	0.361672	0.351098	0.118311
24	157.72	0.123665	0.323833	0.399605	0.152897
25	160.294	0.083383	0.268805	0.437052	0.21076
26	163.278	0.0504098	0.202224	0.448412	0.298954

.TGXKBTH

Example 01

Depropanizer

Iterations = 9; Theta = 1.00024

Component	xD	xB
ethane	0.0145259	7.58589e-011
propane	0.983173	0.0020591
i-butane	0.00204554	0.166455
n-butane	0.000255082	0.416169
n-pentane	6.36716e-009	0.415317

Plate number	T °C	Liquid Compositions				
		ethane	propane	i-butane	n-butane	n-pentane
1	62.302	0.00430205	0.989916	0.00495332	0.000828888	6.02485e-008
2	62.7298	0.00236603	0.986305	0.00933573	0.0019925	3.7931e-007
3	63.0745	0.00199473	0.977776	0.0158921	0.00433448	2.25152e-006
4	63.5637	0.00191241	0.963563	0.0255335	0.00897799	1.30809e-005
5	64.3421	0.00187616	0.940805	0.0392893	0.017955	7.42796e-005
6	65.5925	0.00183619	0.905215	0.0579366	0.0346045	0.00040739
7	67.5779	0.00177765	0.851531	0.0811026	0.0634725	0.00211596
8	70.7056	0.00169075	0.774301	0.105652	0.108256	0.0101001
9	75.7846	0.00156216	0.667863	0.123509	0.164888	0.0421777
10	84.5686	0.00137161	0.527881	0.121139	0.208446	0.141162
11	87.6292	0.000404142	0.475352	0.148311	0.231582	0.144351
12	92.2273	0.000112392	0.397022	0.186844	0.266897	0.149125
13	98.37	2.8998e-005	0.300764	0.231605	0.312447	0.155155
14	105.175	6.90592e-006	0.205263	0.27223	0.361078	0.161423
15	111.356	1.53328e-006	0.127795	0.299892	0.40528	0.167031
16	116.126	3.23035e-007	0.0742067	0.311899	0.44179	0.172103
17	119.499	6.56361e-008	0.0409766	0.309835	0.470874	0.178314
18	122.013	1.29846e-008	0.0217203	0.295665	0.49257	0.190045

19	124.51	2.49958e-009	0.010987	0.269186	0.502185	0.217643
20	128.262	4.59722e-010	0.00514183	0.227177	0.484991	0.28269
21	135.091	7.58589e-011	0.0020591	0.166455	0.416169	0.415317

Example 02

Separation-of-Paraffins

Iterations = 11; Theta = 0.999998

Component	xD	xB
nonane	0.14143	0.0131744
n-decane	0.596272	0.182636
undecane	0.242861	0.234127
n-dodacane	0.0193241	0.211186
n-tridecane	0.000112481	0.206654
n-tetradecane	2.78847e-007	0.152222

Plate number	T °C	Liquid Compositions					
		nonane	n-decane	undecane	n-dodacane	n-tridecane	n-tetradecane
1	166.386	0.0664768	0.508825	0.371679	0.0524778	0.000538905	2.32928e-006
2	169.841	0.0453892	0.434624	0.4301	0.0884724	0.00140434	9.72515e-006
3	172.08	0.0390404	0.386187	0.446406	0.125264	0.00306787	3.48177e-005
4	173.771	0.0365833	0.355701	0.440267	0.161186	0.00614683	0.000116283
5	175.225	0.0352064	0.335219	0.423062	0.194488	0.0116535	0.000370823
6	176.607	0.0341454	0.319658	0.400726	0.223178	0.0211558	0.00113673
7	178.046	0.0331364	0.305942	0.37582	0.244877	0.0368762	0.00334799
8	179.696	0.0320171	0.291854	0.348674	0.256585	0.0614554	0.00941418
9	181.799	0.0306113	0.275255	0.318019	0.254493	0.0967082	0.024914

10	184.708	0.0287144	0.253935	0.28181	0.234632	0.140406	0.0605033
11	188.802	0.0261987	0.226683	0.239276	0.195903	0.181879	0.13006
12	189.152	0.0261444	0.226649	0.239298	0.19593	0.181904	0.130074
13	189.501	0.0260784	0.226622	0.239323	0.195959	0.181929	0.130088
14	189.849	0.0259915	0.226608	0.239353	0.19599	0.181954	0.130103
15	190.198	0.0258671	0.226613	0.239394	0.196025	0.181982	0.130119
16	190.55	0.0256754	0.226651	0.239455	0.196067	0.182015	0.130137
17	190.909	0.0253635	0.22673	0.239564	0.196128	0.182056	0.130158
18	191.285	0.0248356	0.226827	0.239792	0.196238	0.18212	0.130188
19	191.706	0.0239163	0.226732	0.240334	0.196508	0.18226	0.130248
20	192.254	0.0222719	0.225403	0.241652	0.197432	0.18278	0.130461
21	193.293	0.0192133	0.218016	0.243762	0.201067	0.185843	0.132098
22	196.921	0.0131744	0.182636	0.234127	0.211186	0.206654	0.152222

Example 03

Depropanizer

Iterations = 9; Theta = 0.999959

Component	xD	xB
methane	0.434057	2.9246e-015
ethane	0.15025	2.66525e-009
propane	0.415689	0.00249894
n-butane	3.60759e-006	0.423935
n-pentane	2.16046e-011	0.274314
n-hexane	4.204e-016	0.299252

Plate number	T °C	Liquid Compositions					
		methane	ethane	propane	n-butane	n-pentane	n-hexane
1	28.0596	0.0366083	0.0788551	0.884507	2.93716e-005	6.13106e-010	3.96954e-014
2	47.6528	0.0136342	0.0399993	0.946277	8.93452e-005	5.51591e-009	1.04915e-012
3	49.5776	0.0124581	0.0303614	0.956935	0.000245421	4.57968e-008	2.56977e-011
4	49.9031	0.0123765	0.0281318	0.958834	0.000657452	3.75626e-007	6.22066e-010
5	50.0119	0.0123634	0.0276078	0.95828	0.00174591	3.07024e-006	1.50023e-008
6	50.1361	0.0123513	0.0274455	0.955566	0.00461214	2.50043e-005	3.60289e-007
7	50.4176	0.0123224	0.0272928	0.948086	0.0120887	0.000201934	8.56828e-006
8	51.1646	0.0122423	0.0269422	0.927941	0.0310813	0.00159428	0.000198474
9	53.4466	0.0119973	0.0259177	0.870678	0.0754168	0.0117468	0.00424327
10	62.7565	0.0110737	0.0222973	0.68867	0.145755	0.0659692	0.0662347
11	75.6027	0.00077603	0.00693507	0.68693	0.171414	0.0672459	0.0666989
12	80.0358	5.25945e-005	0.00203159	0.633801	0.227014	0.0695941	0.0675073
13	86.5616	3.3982e-006	0.000546405	0.523256	0.332932	0.074194	0.0690685
14	96.8283	2.04346e-007	0.000129282	0.365705	0.481432	0.0813487	0.0713849
15	108.705	1.13638e-008	2.66118e-005	0.213275	0.62254	0.0902995	0.0738592
16	118.552	5.94485e-010	4.91354e-006	0.107935	0.713842	0.101945	0.0762738
17	125.266	2.98858e-011	8.45118e-007	0.0497198	0.748274	0.121534	0.0804713
18	130.583	1.45722e-012	1.37603e-007	0.0212276	0.725219	0.158808	0.094745
19	138.016	6.81444e-014	2.07456e-008	0.00812306	0.623896	0.219842	0.148139
20	152.589	2.9246e-015	2.66525e-009	0.00249894	0.423935	0.274314	0.299252

Example 04

Ethane splitter

Iterations = 9; Theta = 1.0001

Componentt	xD	xB
methane	0.129871	3.29201e-009
ethane	0.86987	0.0245548
propylene	0.00019849	0.243778
propane	6.13407e-005	0.325164
n-butane	1.62413e-008	0.162601
n-pentane	1.53338e-009	0.243902

Plate	T °C	liquid Compositions					
number		methane	ethane	propylene	propane	i-butane	n-butane
1	2.53954	0.0185911	0.980208	0.000869706	0.000330757	2.61754e-007	3.72518e-008
2	5.75017	0.0078404	0.988438	0.00255129	0.00116706	2.55871e-006	5.38848e-007
3	6.29435	0.00682736	0.982494	0.00685084	0.00379603	2.38676e-005	7.49429e-006
4	7.0067	0.0066805	0.963537	0.0175908	0.0118731	0.000216807	0.00010149
5	8.89647	0.00651999	0.912882	0.0424727	0.03499	0.00184999	0.00128564
6	14.0943	0.0061249	0.788985	0.0888107	0.0890981	0.0133597	0.0136211
7	27.83	0.00524594	0.547533	0.131253	0.158904	0.0640247	0.0930398
8	31.1351	0.000845605	0.526909	0.144378	0.169091	0.064876	0.0938999
9	34.7999	0.000131409	0.474329	0.171705	0.191432	0.0666869	0.0957149
10	41.4605	1.91471e-005	0.379464	0.218135	0.232951	0.0702251	0.0992052
11	51.5506	2.54309e-006	0.255816	0.272847	0.289832	0.0763735	0.105129
12	62.903	3.06314e-007	0.143166	0.309557	0.342475	0.0878241	0.116977
13	73.6036	3.37487e-008	0.0668035	0.305092	0.365002	0.112831	0.150271
14	85.6626	3.29175e-009	0.0245533	0.243778	0.325165	0.162602	0.243902

Example 05

Fractionation-of-Xylenes

Iterations = 11; Theta = 0.999984

Component	xD	xB
ethylbenzene	0.0609748	3.6319e-006
p-xylene	0.688784	0.00109411
m-xylene	0.231465	0.00110319
o-xylene	0.018776	0.997799

Plate number	T °C	liquid Compositions			
		E.B	p-xylene	m-xylene	o-xylene
1	138.52	0.0573041	0.685605	0.23509	0.0220002
2	138.696	0.0541151	0.682195	0.238262	0.0254273
3	138.872	0.0513436	0.678582	0.24101	0.0290651
4	139.047	0.0489334	0.674786	0.243359	0.0329212
5	139.222	0.0468353	0.670827	0.245335	0.0370031
6	139.397	0.0450067	0.666717	0.246959	0.0413177
7	139.573	0.0434103	0.662466	0.248253	0.0458715
8	139.748	0.0420137	0.658082	0.249234	0.0506704
9	139.924	0.0407889	0.653571	0.249921	0.0557194
10	140.101	0.0397115	0.648937	0.250329	0.0610227
11	140.278	0.0387604	0.644183	0.250473	0.0665835
12	140.456	0.0379171	0.639311	0.250368	0.0724038
13	140.635	0.0371661	0.634323	0.250027	0.0784842
14	140.814	0.0364935	0.629221	0.249462	0.0848241
15	140.994	0.0358877	0.624006	0.248685	0.0914211
16	141.175	0.0353386	0.618682	0.247708	0.0982713
17	141.357	0.0348373	0.613251	0.246543	0.105369
18	141.54	0.0343766	0.607717	0.2452	0.112707
19	141.723	0.03395	0.602084	0.243691	0.120275
20	141.908	0.0335522	0.596358	0.242027	0.128063
21	142.092	0.0331786	0.590545	0.240219	0.136057
22	142.278	0.0328254	0.584654	0.238279	0.144242
23	142.464	0.0324894	0.578693	0.236217	0.152601
24	142.651	0.0321679	0.572671	0.234045	0.161116
25	142.838	0.0318587	0.5666	0.231774	0.169767
26	143.025	0.0315601	0.560491	0.229416	0.178532
27	143.212	0.0312707	0.554357	0.226983	0.18739
28	143.4	0.0309893	0.54821	0.224486	0.196315
29	143.587	0.0307152	0.542064	0.221936	0.205284
30	143.774	0.0304477	0.535934	0.219346	0.214273

31	143.961	0.0301863	0.529833	0.216725	0.223256
32	144.147	0.0299309	0.523776	0.214086	0.232208
33	144.333	0.0296812	0.517776	0.211438	0.241105
34	144.518	0.0294373	0.511849	0.208791	0.249923
35	144.702	0.0291991	0.506006	0.206156	0.258639
36	144.885	0.0289667	0.500261	0.203542	0.26723
37	145.067	0.0287403	0.494626	0.200956	0.275677
38	145.247	0.02852	0.489112	0.198407	0.28396
39	145.426	0.0283059	0.483729	0.195903	0.292062
40	145.604	0.0280983	0.478487	0.193449	0.299965
41	145.781	0.0278973	0.473393	0.191052	0.307658
42	145.955	0.027703	0.468454	0.188717	0.315126
43	146.129	0.0275156	0.463676	0.186448	0.32236
44	146.3.	0.0273351	0.459065	0.184249	0.329351
45	146.47	0.0271616	0.454623	0.182122	0.336093
46	146.638	0.0269952	0.450353	0.180071	0.342581
47	146.906	0.0245861	0.433604	0.176615	0.365194
48	147.183	0.0223106	0.415934	0.172576	0.38918
49	147.466	0.0201683	0.397433	0.167965	0.414433
50	147.756	0.0181591	0.378219	0.162807	0.440815
51	148.051	0.0162828	0.358428	0.157138	0.468151
52	148.351	0.0145386	0.338214	0.151007	0.49624
53	148.654	0.0129255	0.317745	0.144473	0.524856
54	148.958	0.0114414	0.2972	0.137605	0.553754
55	149.263	0.0100838	0.276756	0.130477	0.582683
56	149.566	0.00884896	0.25659	0.12317	0.611391
57	149.867	0.00773245	0.236869	0.115764	0.639634
58	150.163	0.0067289	0.217746	0.108341	0.667185
59	150.454	0.0058322	0.199352	0.100975	0.693841
60	150.738	0.00503561	0.1818	0.0937379	0.719426
61	151.015	0.00433195	0.165177	0.086691	0.7438
62	151.284	0.00371377	0.149546	0.0798877	0.766852
63	151.544	0.0031735	0.134948	0.0733711	0.788508
64	151.795	0.00270365	0.121398	0.0671749	0.808723
65	152.037	0.00229692	0.108897	0.0613228	0.827483
66	152.27	0.00194636	0.097426	0.05583	0.844798
67	152.494	0.00164541	0.0869518	0.0507034	0.860699
68	152.709	0.00138801	0.0774318	0.0459434	0.875237
69	152.915	0.00116859	0.0688152	0.0415442	0.888472
70	153.114	0.000982123	0.0610456	0.0374957	0.900477
71	153.305	0.000824102	0.0540636	0.0337841	0.911328
72	153.49	0.000690522	0.0478088	0.0303929	0.921108

73	153.668	0.000577858	0.0422207	0.0273041	0.929897
74	153.84	0.000483026	0.0372407	0.0244982	0.937778
75	154.006	0.000403349	0.0328123	0.0219556	0.944829
76	154.167	0.000336512	0.0288822	0.0196565	0.951125
77	154.324	0.000280526	0.0254002	0.0175817	0.956738
78	154.477	0.000233687	0.0223202	0.0157125	0.961734
79	154.626	0.000194546	0.0195993	0.014031	0.966175
80	154.771	0.000161868	0.0171985	0.0125203	0.970119
81	154.913	0.00013461	0.0150826	0.0111648	0.973618
82	155.053	0.000111891	0.0132193	0.00994967	0.976719
83	155.19	9.29657e-005	0.0115799	0.00886143	0.979466
84	155.325	7.72107e-005	0.0101384	0.00788761	0.981897
85	155.457	6.4101e-005	0.00887181	0.00701676	0.984047
86	155.588	5.31973e-005	0.00775947	0.00623848	0.985949
87	155.717	4.41314e-005	0.00678304	0.0055433	0.98763
88	155.845	3.65961e-005	0.00592627	0.00492264	0.989114
89	155.971	3.03345e-005	0.00517476	0.00436872	0.990426
90	156.097	2.51325e-005	0.00451577	0.00387455	0.991585
91	156.221	2.08116e-005	0.00393807	0.00343382	0.992607
92	156.343	1.72231e-005	0.00343172	0.00304084	0.99351
93	156.465	1.42431e-005	0.00298801	0.00269052	0.994307
94	156.587	1.17689e-005	0.00259924	0.00237829	0.995011
95	156.707	9.71457e-006	0.00225865	0.00210006	0.995632
96	156.827	8.00906e-006	0.00196031	0.00185215	0.99618
97	156.946	6.59318e-006	0.00169899	0.00163129	0.996663
98	157.064	5.41776e-006	0.00147011	0.00143454	0.99709
99	157.182	4.44197e-006	0.00126966	0.00125929	0.997467
100	157.299	3.6319e-006	0.00109411	0.00110319	0.997799

Example 06

Separation of Ethylbenzene-Styrene

Iterations = 14 ; Theta = 1.00001

Component	xD	xB
benzene	0.022	1.96541e-017
ethylbenzene	0.962524	0.0774771
styrene	0.0154668	0.914532
i-propylbenzene	9.39503e-006	0.0079906

Plate number	T °C	liquid Compositions			
		toluene	E.B	styrene	i-propylebenzene
1	57.5126	0.00874397	0.969028	0.0222125	1.58626e-005
2	59.0355	0.00412211	0.965544	0.0303091	2.50887e-005
3	60.4067	0.00252083	0.957403	0.040038	3.82185e-005
4	61.7011	0.00196769	0.946306	0.0516692	5.67954e-005

5	62.9491	0.00177717	0.932683	0.0654573	8.28751e-005
6	64.165	0.00171136	0.916539	0.0816302	0.000119156
7	65.3573	0.00168749	0.897775	0.100368	0.000169115
8	66.5313	0.00167676	0.876308	0.121778	0.000237142
9	67.6909	0.00166914	0.852139	0.145863	0.000328648
10	68.8386	0.00166121	0.825389	0.172499	0.000450139
11	69.9751	0.00165193	0.796322	0.201417	0.000609233
12	71.1003	0.00164116	0.76535	0.232195	0.000814619
13	72.2122	0.00162912	0.733018	0.264277	0.00107596
14	73.3081	0.0016162	0.699973	0.297007	0.0014038
15	74.3843	0.00160285	0.666912	0.329676	0.00180942
16	75.437	0.00158955	0.634527	0.361579	0.00230486
17	76.2658	0.000685672	0.633878	0.363124	0.00231189
18	77.055	0.00029645	0.63281	0.364575	0.00231825
19	77.8173	0.00012849	0.631523	0.366024	0.00232439
20	78.559	5.58319e-005	0.630089	0.367525	0.00233053
21	79.2832	2.43201e-005	0.628524	0.369115	0.00233681
22	79.992	1.06189e-005	0.626816	0.37083	0.00234332
23	80.6868	4.64709e-006	0.624938	0.372707	0.00235017
24	81.3689	2.03805e-006	0.622851	0.374789	0.00235748
25	82.0393	8.95615e-007	0.620504	0.377129	0.00236538
26	82.6991	3.94311e-007	0.617838	0.379788	0.00237401
27	83.3497	1.73898e-007	0.614778	0.382839	0.00238358
28	83.9922	7.6809e-008	0.611236	0.386369	0.00239429
29	84.628	3.39701e-008	0.60711	0.390484	0.00240642
30	85.2586	1.504e-008	0.602277	0.395303	0.00242028
31	85.8855	6.66419e-009	0.596596	0.400968	0.00243625
32	86.5104	2.95433e-009	0.589905	0.40764	0.00245477
33	87.1355	1.30988e-009	0.582021	0.415502	0.00247635
34	87.7626	5.80606e-010	0.572744	0.424754	0.00250159
35	88.394	2.57166e-010	0.561858	0.435611	0.00253118
36	89.032	1.13763e-010	0.549141	0.448293	0.00256592
37	89.6788	5.02336e-011	0.534374	0.463019	0.00260671
38	90.3367	2.21268e-011	0.51736	0.479985	0.0026546
39	91.0075	9.71594e-012	0.497941	0.499348	0.00271081
40	91.6926	4.24998e-012	0.476025	0.521199	0.00277674
41	92.3927	1.85063e-012	0.451606	0.54554	0.00285411
42	93.1076	8.01655e-013	0.424791	0.572264	0.00294503
43	93.8362	3.45237e-013	0.395813	0.601134	0.00305222
44	94.576	1.47732e-013	0.365039	0.631782	0.00317921
45	95.3234	6.27886e-014	0.332951	0.663719	0.00333075
46	96.074	2.64982e-014	0.300127	0.69636	0.00351322
47	96.8226	1.11028e-014	0.267199	0.729066	0.0037352
48	97.5639	4.61883e-015	0.234799	0.761192	0.0040082
49	98.2926	1.90789e-015	0.20352	0.792133	0.00434747
50	99.0041	7.82517e-016	0.173865	0.821362	0.00477309
51	99.6948	3.18526e-016	0.146228	0.848461	0.00531123
52	100.362	1.2844e-016	0.120874	0.873131	0.00599578
53	101.004	5.10201e-017	0.0979458	0.895184	0.00687029
54	101.621	1.96541e-017	0.0774771	0.914532	0.0079906

Example 07

Seperation-of-Toluene_Ethyl-benzene

Iterations = 13; Theta = 1

Component	xD	Xb
benzene	0.364695	0.00174755
toluene	0.485691	0.0496701
ethylbenzene	0.126954	0.452146
styrene	0.0226599	0.496437

Plate number	T °C	liquid Compositions			
		benzene	toluene	E.B	styrene
1	63.8349	0.130396	0.481377	0.310188	0.0780396
2	73.5801	0.0458526	0.338503	0.459472	0.156172
3	79.8342	0.0231987	0.20981	0.527883	0.239108
4	83.625	0.0173606	0.133993	0.531075	0.317571
5	85.9862	0.0155663	0.0962724	0.498208	0.389953
6	87.606	0.0148311	0.0785786	0.449808	0.456782
7	88.7363	0.0101523	0.0774417	0.453029	0.459377
8	89.8248	0.00653697	0.0738965	0.456446	0.46312
9	90.9939	0.0037931	0.0658851	0.45898	0.471342
10	92.5063	0.00174755	0.0496701	0.452146	0.496437

Example 08

Biphenyl-separation

Iterations = 8; Theta = 0.999646

Component	xD	xB
benzene	0.950531	1.46259e-005
toluene	0.0494687	0.0165737
biphenyl	4.35725e-007	0.983412

Plate number	T °C	Liquid Compositions		
		benzene	toluene	diphenyl
1	95.7935	0.886448	0.113545	7.26452e-006
2	97.4327	0.821489	0.17845	6.09609e-005
3	99.0328	0.761144	0.238393	0.000462428
4	100.548	0.708108	0.288565	0.00332746
5	102.379	0.65555	0.321841	0.0226089
6	108.496	0.452472	0.524413	0.0231146
7	115.135	0.265102	0.711301	0.023597
8	120.407	0.1371	0.838839	0.0240606
9	123.729	0.0657584	0.908975	0.0252664
10	125.749	0.0301909	0.937597	0.032212
11	128.161	0.0131562	0.911899	0.0749449

12	136.718	0.00475082	0.718448	0.276801
13	162.084	0.00102658	0.318598	0.680376
14	190.524	0.000134502	0.0806987	0.919167
15	202.259	1.46259e-005	0.0165737	0.983412

Example 09

Phenol-Cresol-separation

Iterations = 8 Theta = 1

Component	xD	xB
phenol	0.955518	0.0504089
o-cresol	0.0444451	0.202225
m-cresol	3.69887e-005	0.448412
2,3 xylenol	1.17385e-008	0.298954

Plate number	T °C	liquid Compositions			
		phenol	o-cresol	m-cresol	2,3 xylenol
1	131.532	0.9436	0.0563294	7.10261e-005	3.49058e-008
2	132.322	0.930076	0.0697942	0.000129858	9.69707e-008
3	133.108	0.914823	0.0849462	0.000230963	2.6216e-007
4	133.893	0.89773	0.101866	0.000403643	6.98791e-007
5	134.679	0.878707	0.120595	0.000696604	1.84439e-006
6	135.467	0.857684	0.141121	0.00119002	4.82638e-006
7	136.259	0.834612	0.163361	0.00201443	1.25223e-005
8	137.059	0.809452	0.187136	0.00337981	3.21999e-005
9	137.871	0.782155	0.212144	0.00561897	8.20032e-005
10	138.701	0.75263	0.237914	0.00924996	0.000206627
11	139.559	0.720682	0.263743	0.0150601	0.000514431
12	140.462	0.685935	0.288597	0.0242055	0.00126296
13	141.438	0.647712	0.310945	0.0382953	0.0030483
14	142.536	0.604899	0.328539	0.0593638	0.00719879
15	143.833	0.55585	0.338138	0.0895042	0.0165078
16	145.451	0.498533	0.335409	0.129738	0.0363202
17	147.56	0.431387	0.31559	0.177703	0.0753189
18	148.537	0.39482	0.338731	0.189708	0.0767409
19	149.606	0.354504	0.359928	0.206705	0.0788639
20	150.795	0.310813	0.376499	0.230402	0.0822866
21	152.146	0.264457	0.384961	0.262387	0.0881954
22	153.708	0.216593	0.381292	0.303256	0.0988588
23	155.544	0.168917	0.361674	0.351098	0.118311
24	157.72	0.123663	0.323835	0.399605	0.152897
25	160.294	0.0833815	0.268806	0.437053	0.21076
26	163.278	0.0504089	0.202225	0.448412	0.298954

TGCKBTTH

Example 01

Depropanizer

Iterations = 9; Theta = 1.00015

Component	xD	xB
ethane	0.0145259	7.5745e-011
propane	0.983175	0.00205759
i-butane	0.00204432	0.166456
n-butane	0.000254832	0.41617
n-pentane	6.35563e-009	0.415317

Plate	T °C	liquid Compositions				
number		ethane	propane	i-butane	n-butane	n-pentane
1	62.286	0.00430175	0.989919	0.00495059	0.000828136	6.01481e-008
2	62.7136	0.0023658	0.986312	0.00933098	0.00199082	3.78731e-007
3	63.0579	0.00199455	0.977787	0.0158847	0.00433113	2.24843e-006
4	63.5467	0.00191224	0.96358	0.0255229	0.00897176	1.30651e-005
5	64.3244	0.00187599	0.94083	0.0392755	0.0179442	7.42028e-005
6	65.5739	0.00183602	0.905249	0.0579205	0.0345874	0.000407048
7	67.5583	0.00177748	0.851572	0.0810871	0.0634488	0.00211462
8	70.6852	0.00169056	0.774341	0.105642	0.10823	0.0100959
9	75.7642	0.00156196	0.667891	0.123509	0.164869	0.0421693
10	84.5494	0.0013714	0.527883	0.121146	0.208441	0.141158
11	87.6107	0.000404042	0.475342	0.148328	0.231581	0.144344
12	92.2109	0.00011235	0.39699	0.186875	0.266905	0.149118
13	98.3563	2.89833e-005	0.300713	0.231646	0.312463	0.155148
14	105.162	6.90139e-006	0.205206	0.272273	0.361096	0.161417
15	111.343	1.53205e-006	0.127747	0.299929	0.405295	0.167027
16	116.111	3.22733e-007	0.0741728	0.311928	0.4418	0.172099
17	119.483	6.55668e-008	0.040955	0.309857	0.47088	0.178309
18	121.996	1.29694e-008	0.0217076	0.295681	0.492573	0.190038

19	124.492	2.49638e-009	0.0109801	0.269197	0.502188	0.217635
20	128.244	4.59083e-010	0.00513832	0.227183	0.484995	0.282683
21	135.072	7.5745e-011	0.00205759	0.166456	0.41617	0.415317

Example 02

Separation-of-Paraffins

Iterations = 11; Theta = 0.999998

Component	xD	xB
nonane	0.141621	0.0131532
n-decane	0.5966	0.1826
undecane	0.242577	0.234158
n-dodacne	0.0190917	0.211212
n-tridecane	0.000109523	0.206655
n-tetradecane	2.6888e-007	0.152222

Plate	T °C	Liquid Compositions					
number		nonane	n-decane	undecane	n-dodacane	n-tridecane	n-tetradecane
1	166.015	0.0665349	0.50929	0.371693	0.0519539	0.000526294	2.25465e-006
2	169.469	0.0454206	0.435075	0.430405	0.0877147	0.00137471	9.44484e-006
3	171.706	0.0390674	0.386602	0.446928	0.124358	0.0030105	3.39321e-005
4	173.398	0.0366097	0.356084	0.440917	0.160229	0.00604719	0.000113729
5	174.852	0.0352322	0.335573	0.423758	0.193578	0.0114943	0.000363971
6	176.236	0.0341701	0.319983	0.401405	0.222401	0.0209207	0.00111964
7	177.676	0.0331596	0.306235	0.376436	0.2443	0.0365598	0.003309
8	179.329	0.032038	0.292111	0.349194	0.256242	0.0610797	0.00933548
9	181.435	0.0306287	0.275463	0.318414	0.254368	0.0963433	0.0247838
10	184.349	0.0287254	0.254065	0.28204	0.234643	0.140168	0.060359

11	188.455	0.0261992	0.226695	0.239297	0.195904	0.181858	0.130047
12	188.808	0.0261443	0.226661	0.23932	0.195932	0.181882	0.130061
13	189.159	0.0260776	0.226634	0.239345	0.195961	0.181907	0.130076
14	189.51	0.0259899	0.226619	0.239375	0.195992	0.181934	0.130091
15	189.861	0.0258644	0.226625	0.239416	0.196027	0.181962	0.130106
16	190.215	0.0256713	0.226662	0.239478	0.19607	0.181994	0.130124
17	190.576	0.0253574	0.226742	0.239588	0.196131	0.182036	0.130145
18	190.955	0.024827	0.22684	0.239816	0.196241	0.1821	0.130176
19	191.378	0.0239043	0.226746	0.240361	0.196512	0.182241	0.130236
20	191.929	0.0222557	0.225416	0.241682	0.197437	0.182761	0.130448
21	192.97	0.0191932	0.21802	0.2438	0.201078	0.185825	0.132085
22	196.602	0.0131532	0.1826	0.234158	0.211212	0.206655	0.152222

Example 03

Depropanizer

Iterations = 9 Theta = 0.999918

Component	xD	xB
methane	0.434057	2.91997e-015
ethane	0.15025	2.66339e-009
propane	0.415689	0.00249882
n-butane	3.6053e-006	0.423935
n-pentane	2.15788e-011	0.274314
n-hexane	4.19655e-016	0.299252

Plate number	T °C	Liquid Compositions					
		methane	ethane	propane	n-butane	n-pentane	n-hexane
1	28.0476	0.0366024	0.0788505	0.884518	2.93553e-005	6.12469e-010	3.96339e-014
2	47.6441	0.0136321	0.039996	0.946283	8.92992e-005	5.51067e-009	1.04767e-012
3	49.5667	0.0124566	0.0303594	0.956939	0.000245306	4.57579e-008	2.56653e-011
4	49.8907	0.0123749	0.0281302	0.958837	0.000657175	3.75349e-007	6.2139e-010
5	49.9991	0.0123615	0.027606	0.958284	0.00174527	3.06836e-006	1.49888e-008
6	50.1234	0.0123493	0.0274432	0.955571	0.00461077	2.49923e-005	3.60034e-007
7	50.4054	0.0123203	0.0272903	0.948093	0.0120859	0.000201863	8.56386e-006
8	51.1526	0.0122402	0.0269398	0.927951	0.0310763	0.00159392	0.000198408
9	53.4346	0.0119954	0.0259155	0.870691	0.0754098	0.0117456	0.00424266
10	62.7441	0.011072	0.0222954	0.688676	0.14575	0.0659701	0.0662362
11	75.5884	0.000775804	0.00693415	0.686944	0.1714	0.0672463	0.0667002
12	80.0202	5.25723e-005	0.00203124	0.633828	0.226986	0.0695936	0.0675082
13	86.5444	3.39634e-006	0.000546295	0.523298	0.332892	0.0741922	0.0690687
14	96.8102	2.04208e-007	0.000129251	0.365746	0.481394	0.0813458	0.0713844
15	108.687	1.13545e-008	2.66043e-005	0.213301	0.622518	0.0902958	0.0738582
16	118.535	5.93913e-010	4.91181e-006	0.107947	0.713836	0.10194	0.0762724
17	125.25	2.98525e-011	8.44754e-007	0.0497238	0.748278	0.121529	0.0804691
18	130.567	1.45537e-012	1.37533e-007	0.0212286	0.725228	0.158802	0.0947412
19	137.999	6.80473e-014	2.07331e-008	0.00812309	0.623905	0.219838	0.148134
20	152.573	2.91997e-015	2.66339e-009	0.00249882	0.423935	0.274314	0.299252

Example 04
Ethane-splitter
Iterations = 10; Theta = 1.00002

Component	xD	xB
methane	0.12987	3.28883e-009
ethane	0.86987	0.0245532
propylene	0.000198382	0.243778
propane	6.13037e-005	0.325165
i-butane	1.62257e-008	0.162602
n-butane	1.53162e-009	0.243902

Plate	T °C	Liquid Compositions					
number		methane	ethane	propylene	propane	i-butane	n-butane
1	2.52873	0.0185891	0.980211	0.000869267	0.000330575	2.61533e-007	3.72143e-008
2	5.73917	0.00783937	0.988441	0.00255016	0.0011665	2.55687e-006	5.38388e-007
3	6.2832	0.00682654	0.982499	0.00684826	0.0037945	2.38536e-005	7.48908e-006
4	6.99532	0.00667973	0.963547	0.0175855	0.0118693	0.000216709	0.000101436
5	8.88462	0.00651926	0.912901	0.0424634	0.0349821	0.00184942	0.00128518
6	14.0817	0.00612424	0.789012	0.0887997	0.0890872	0.0133577	0.0136188
7	27.8168	0.00524535	0.547548	0.131246	0.158898	0.0640238	0.0930386
8	31.1212	0.000845424	0.526931	0.144369	0.169082	0.0648748	0.0938984
9	34.7852	0.000131369	0.474358	0.171692	0.19142	0.0666853	0.0957131
10	41.4451	1.91393e-005	0.379496	0.218121	0.232937	0.0702231	0.099203
11	51.535	2.5418e-006	0.25584	0.272839	0.289821	0.0763714	0.105126
12	62.888	3.06123e-007	0.143178	0.309556	0.342471	0.0878219	0.116974
13	73.5892	3.37234e-008	0.0668065	0.305094	0.365003	0.112829	0.150268
14	85.6483	3.28883e-009	0.0245532	0.243778	0.325165	0.162602	0.243902

Example 05

Fractionation-of-Xylenes

Iterations = 11; Theta = 0.999984

Component	xD	xB
ethylbenzene	0.0609748	3.60382e-006
p-xylene	0.688786	0.00108721
m-xylene	0.231466	0.00109766
o-xylene	0.0187733	0.997812

Plate number	T °C	Liquid Compositions			
		E.B	p-xylene	m-xylene	o-xylene
1	138.372	0.0573019	0.685602	0.235097	0.021999
2	138.549	0.0541111	0.682188	0.238273	0.0254279
3	138.725	0.051338	0.678569	0.241025	0.0290679
4	138.901	0.0489265	0.674769	0.243378	0.0329267
5	139.076	0.0468275	0.670804	0.245356	0.0370118
6	139.252	0.044998	0.666689	0.246983	0.04133
7	139.428	0.0434009	0.662432	0.248279	0.045888
8	139.604	0.0420038	0.658043	0.249262	0.0506915
9	139.78	0.0407786	0.653526	0.24995	0.0557458
10	139.957	0.0397008	0.648886	0.250358	0.061055
11	140.135	0.0387493	0.644125	0.250503	0.0666224
12	140.314	0.0379058	0.639247	0.250398	0.0724498
13	140.493	0.0371545	0.634252	0.250055	0.078538
14	140.673	0.0364818	0.629143	0.249489	0.0848864
15	140.853	0.0358757	0.623921	0.24871	0.0914925
16	141.035	0.0353264	0.61859	0.247732	0.0983524
17	141.217	0.0348249	0.613151	0.246564	0.10546
18	141.4	0.034364	0.607608	0.245218	0.112809
19	141.584	0.0339372	0.601967	0.243706	0.120389
20	141.769	0.0335392	0.596233	0.242039	0.128189
21	141.954	0.0331654	0.590412	0.240227	0.136195
22	142.14	0.032812	0.584512	0.238283	0.144393
23	142.327	0.0324758	0.578542	0.236217	0.152765
24	142.514	0.032154	0.572512	0.23404	0.161294
25	142.701	0.0318446	0.566432	0.231765	0.169958
26	142.889	0.0315458	0.560314	0.229403	0.178737
27	143.077	0.0312561	0.554171	0.226965	0.187608
28	143.264	0.0309745	0.548015	0.224463	0.196547
29	143.452	0.0307001	0.541861	0.221909	0.20553
30	143.64	0.0304324	0.535723	0.219313	0.214532

31	143.827	0.0301708	0.529614	0.216688	0.223527
32	144.014	0.0299152	0.523549	0.214044	0.232492
33	144.2	0.0296653	0.517543	0.211391	0.241401
34	144.385	0.0294212	0.511608	0.20874	0.25023
35	144.569	0.0291828	0.505759	0.206101	0.258957
36	144.753	0.0289503	0.500009	0.203483	0.267558
37	144.935	0.0287237	0.494368	0.200893	0.276015
38	145.116	0.0285033	0.488849	0.198341	0.284306
39	145.296	0.0282891	0.483462	0.195834	0.292415
40	145.474	0.0280814	0.478216	0.193377	0.300326
41	145.651	0.0278803	0.473118	0.190977	0.308024
42	145.826	0.027686	0.468177	0.18864	0.315498
43	146	0.0274985	0.463397	0.186368	0.322736
44	146.171	0.027318	0.458784	0.184167	0.329731
45	146.341	0.0271445	0.45434	0.182039	0.336476
46	146.51	0.0269781	0.450069	0.179987	0.342966
47	146.779	0.0245676	0.433291	0.17652	0.365621
48	147.056	0.0222909	0.415591	0.172469	0.389649
49	147.34	0.0201477	0.397062	0.167846	0.414944
50	147.63	0.0181379	0.377821	0.162677	0.441365
51	147.926	0.0162613	0.358005	0.156996	0.468737
52	148.226	0.0145171	0.33777	0.150854	0.496858
53	148.529	0.0129042	0.317285	0.14431	0.525501
54	148.834	0.0114206	0.296726	0.137433	0.55442
55	149.139	0.0100637	0.276274	0.130298	0.583365
56	149.443	0.00882974	0.256104	0.122984	0.612082
57	149.744	0.00771426	0.236384	0.115575	0.640327
58	150.04	0.00671185	0.217266	0.108149	0.667873
59	150.332	0.00581635	0.198882	0.100783	0.694519
60	150.616	0.00502102	0.181343	0.0935471	0.720089
61	150.893	0.00431862	0.164737	0.0865032	0.744441
62	151.162	0.00370168	0.149125	0.0797043	0.767469
63	151.422	0.00316262	0.134547	0.0731934	0.789097
64	151.673	0.00269391	0.121021	0.0670039	0.809281
65	151.915	0.00228826	0.108544	0.0611595	0.828009
66	152.148	0.00193871	0.097096	0.0556748	0.84529
67	152.372	0.00163868	0.0866458	0.0505569	0.861159
68	152.587	0.00138212	0.0771494	0.0458057	0.875663
69	152.794	0.00116345	0.0685557	0.0414155	0.888865
70	152.993	0.000977663	0.0608081	0.0373758	0.900838
71	153.184	0.000820242	0.0538471	0.0336729	0.91166
72	153.369	0.000687193	0.0476119	0.0302902	0.921411

73	153.547	0.000574994	0.0420424	0.0272094	0.930173
74	153.719	0.00048057	0.0370795	0.0244112	0.938029
75	153.885	0.000401247	0.032667	0.0218759	0.945056
76	154.047	0.000334717	0.0287514	0.0195838	0.95133
77	154.204	0.000278995	0.0252829	0.0175154	0.956923
78	154.357	0.000232385	0.022215	0.0156521	0.961901
79	154.506	0.000193439	0.0195052	0.013976	0.966325
80	154.651	0.000160929	0.0171145	0.0124705	0.970254
81	154.794	0.000133815	0.0150076	0.0111196	0.973739
82	154.934	0.000111217	0.0131525	0.00990883	0.976827
83	155.071	9.23962e-005	0.0115204	0.00882454	0.979563
84	155.206	7.67297e-005	0.0100856	0.00785431	0.981983
85	155.339	6.36951e-005	0.00882492	0.00698675	0.984125
86	155.47	5.2855e-005	0.00771787	0.00621146	0.986018
87	155.599	4.38431e-005	0.00674618	0.005519	0.987691
88	155.727	3.63534e-005	0.00589364	0.0049008	0.989169
89	155.854	3.01304e-005	0.0051459	0.00434912	0.990475
90	155.979	2.4961e-005	0.00449027	0.00385697	0.991628
91	156.103	2.06676e-005	0.00391555	0.00341806	0.992646
92	156.226	1.71023e-005	0.00341187	0.00302674	0.993544
93	156.349	1.4142e-005	0.00297053	0.00267792	0.994337
94	156.47	1.16842e-005	0.00258386	0.00236704	0.995037
95	156.591	9.64379e-006	0.00224514	0.00209002	0.995655
96	156.711	7.94999e-006	0.00194845	0.00184322	0.9962
97	156.83	6.54396e-006	0.0016886	0.00162334	0.996682
98	156.948	5.37683e-006	0.00146103	0.00142749	0.997106
99	157.066	4.40802e-006	0.00126173	0.00125304	0.997481
100	157.184	3.60382e-006	0.00108721	0.00109766	0.997812

Example 06

Iterations = 14; Theta = 1.00001

Component	xD	xB
benzene	0.022	1.79735e-017
ethylbenzene	0.963004	0.0769966
styrene	0.0149869	0.915012
i-propylbenzene	9.03158e-006	0.00799096

Plate number	T °C	Liquid Compositions			
		toluene	E.B	styrene	i-propylebenzene
1	56.1325	0.00869256	0.969706	0.0215863	1.53015e-005
2	57.7211	0.00408157	0.966367	0.0295275	2.42726e-005
3	59.1509	0.00249377	0.958376	0.0390935	3.70772e-005
4	60.4982	0.00194877	0.947439	0.0505575	5.52453e-005
5	61.7941	0.00176251	0.933977	0.0641798	8.08217e-005
6	63.0538	0.00169891	0.917989	0.0801957	0.000116498
7	64.2861	0.00167631	0.899364	0.0987943	0.000165752
8	65.497	0.00166641	0.878008	0.120093	0.000232989
9	66.6908	0.0016594	0.853912	0.144105	0.000323652
10	67.8703	0.00165197	0.827186	0.170718	0.0004443
11	69.0369	0.00164311	0.798088	0.199666	0.000602632
12	70.1903	0.00163268	0.767025	0.230534	0.000807443
13	71.3292	0.00162092	0.734546	0.262765	0.00106853
14	72.4508	0.00160822	0.701302	0.295693	0.00139656
15	73.5515	0.00159504	0.668002	0.3286	0.00180298
16	74.6277	0.00158187	0.635352	0.360766	0.00229998
17	75.4772	0.000680249	0.634679	0.362334	0.00230713
18	76.2859	0.000293224	0.633587	0.363806	0.0023136
19	77.0668	0.000126723	0.632278	0.365275	0.00231985
20	77.8261	5.49085e-005	0.630824	0.366795	0.00232609
21	78.567	2.38523e-005	0.629241	0.368403	0.00233246
22	79.2917	1.03869e-005	0.627517	0.370134	0.00233907
23	80.0016	4.53374e-006	0.625623	0.372026	0.00234601
24	80.698	1.98331e-006	0.623521	0.374124	0.0023534
25	81.3822	8.69412e-007	0.621161	0.376477	0.00236137
26	82.0552	3.81854e-007	0.61848	0.379149	0.00237009
27	82.7183	1.68009e-007	0.615407	0.382213	0.00237972
28	83.3728	7.40376e-008	0.611852	0.385757	0.00239051
29	84.0201	3.26709e-008	0.607711	0.389886	0.00240271
30	84.6617	1.4433e-008	0.602862	0.394721	0.00241664
31	85.2992	6.38147e-009	0.597163	0.400405	0.00243269
32	85.9344	2.82302e-009	0.59045	0.407099	0.00245129
33	86.5693	1.24905e-009	0.582539	0.414988	0.00247296
34	87.206 5	.52514e-010	0.573229	0.424273	0.0024983
35	87.8466	2.44229e-010	0.562302	0.43517	0.00252801
36	88.4936	1.07824e-010	0.549535	0.447902	0.00256289
37	89.1492	4.7517e-011	0.534708	0.462688	0.00260384
38	89.8156	2.0889e-011	0.517621	0.479727	0.00265192
39	90.4948	9.15438e-012	0.498118	0.499173	0.00270834
40	91.1881	3.99647e-012	0.476105	0.52112	0.0027745

41	91.8962	1.73681e-012	0.45158	0.545568	0.00285213
42	92.6191	7.50856e-013	0.424653	0.572404	0.00294333
43	93.3553	3.22714e-013	0.39556	0.601389	0.0030508
44	94.1025	1.37816e-013	0.364673	0.632149	0.00317808
45	94.8571	5.84554e-014	0.332482	0.664188	0.0033299
46	95.6146	2.46192e-014	0.299571	0.696916	0.00351261
47	96.3698	1.02944e-014	0.266575	0.72969	0.00373481
48	97.1172	4.27376e-015	0.234132	0.76186	0.00400798
49	97.8517	1.76176e-015	0.202833	0.79282	0.00434738
50	98.5687	7.2112e-016	0.173183	0.822044	0.00477309
51	99.2644	2.9295e-016	0.145573	0.849116	0.0053113
52	99.9363	1.17896e-016	0.120264	0.87374	0.0059959
53	100.583	4.67434e-017	0.097396	0.895733	0.00687049
54	101.204	1.79735e-017	0.0769966	0.915012	0.00799096

Example 07

Seperation-of-Toluene_Ethyl-benzene

Iterations = 13; Theta = 1

Component	xD	Xb
benzene	0.365039	0.00172722
toluene	0.486764	0.0496066
ethylbenzene	0.125869	0.45221
styrene	0.0223276	0.496456

Plate number	T °C	Liquid Compositions			
		benzene	toluene	E.B	styrene
1	63.2945	0.130481	0.483388	0.308834	0.0772969
2	73.0364	0.0458396	0.340153	0.458742	0.155265
3	79.3075	0.0231651	0.210694	0.527835	0.238306
4	83.1177	0.0173225	0.134359	0.531324	0.316994
5	85.4939	0.0155261	0.0963939	0.498443	0.389637
6	87.125	0.0147901	0.0786022	0.449874	0.456734
7	88.2642	0.0101003	0.0774549	0.453108	0.459337
8	89.3598	0.00648873	0.0738893	0.456535	0.463087
9	90.535	0.00375697	0.0658494	0.459072	0.471322
10	92.0527	0.00172722	0.0496066	0.45221	0.496456

Example 08

Biphenyl-separation

Iterations = 8; Theta = 0.999541

Component	xD	xB
benzene	0.950531	1.45548e-005
toluene	0.0494688	0.0165717
biphnyl	4.34508e-007	0.983414

Plate number	T °C	Liquid Compositions		
		benzene	toluene	diphenyl
1	95.6669	0.886405	0.113588	7.24937e-006
2	97.3072	0.821387	0.178552	6.08708e-005
3	98.9086	0.760979	0.238559	0.000462008
4	100.425	0.707889	0.288784	0.00332617
5	102.257	0.655296	0.322094	0.0226107
6	108.377	0.452097	0.524786	0.0231166
7	115.016	0.264736	0.711665	0.023599
8	120.285	0.136836	0.839102	0.024062
9	123.602	0.0655996	0.909135	0.025265
10	125.618	0.0301051	0.937699	0.032196
11	128.025	0.0131144	0.912027	0.0748583
12	136.567	0.00473501	0.718724	0.276541
13	161.911	0.00102299	0.318791	0.680186
14	190.351	0.000133952	0.0807268	0.919139
15	202.09	1.45548e-005	0.0165717	0.983414

Example 09

Phenol-Cresol-Separation

Iterations = 8; Theta = 1

Component	xD	xB
phenol	0.955609	0.0503638
o-cresol	0.0443549	0.20227
m-cresol	3.61728e-005	0.448413
2,3 xylenol	1.1308e-008	0.298954

Plate number	T °C	Liquid Compositions			
		phenol	o-cresol	m-cresol	2,3 xylenol
1	130.808	0.943703	0.0562279	6.95534e-005	3.37118e-008
2	131.613	0.93019	0.0696825	0.000127326	9.38795e-008
3	132.414	0.914947	0.084826	0.000226739	2.54404e-007
4	133.213	0.897863	0.101739	0.000396747	6.797e-007
5	134.011	0.878848	0.120464	0.000685538	1.79812e-006
6	134.812	0.857832	0.14099	0.00117253	4.71586e-006
7	135.616	0.834767	0.163234	0.00198723	1.22624e-005
8	136.428	0.809613	0.187018	0.00333817	3.15995e-005
9	137.25	0.782323	0.21204	0.00555634	8.0644e-005
10	138.09	0.752808	0.237831	0.00915769	0.000203622
11	138.957	0.720874	0.263691	0.0149275	0.000507984
12	139.869	0.686145	0.288585	0.0240208	0.00124964
13	140.853	0.647944	0.310985	0.0380485	0.00302215
14	141.958	0.605156	0.328641	0.059052	0.00715111
15	143.261	0.556122	0.338306	0.0891414	0.0164304
16	144.886	0.49879	0.335627	0.129364	0.0362178
17	147.001	0.431575	0.315808	0.17738	0.0752367
18	147.985	0.394998	0.339008	0.189341	0.0766533
19	149.059	0.354671	0.36027	0.206291	0.078768
20	150.255	0.310967	0.376909	0.229946	0.0821786
21	151.611	0.264591	0.385429	0.261909	0.0880704
22	153.178	0.216699	0.381789	0.302799	0.0987131
23	155.02	0.168984	0.362149	0.35072	0.118148
24	157.203	0.123685	0.324217	0.399361	0.152737
25	159.783	0.0833622	0.269032	0.436957	0.210648
26	162.775	0.0503638	0.20227	0.448413	0.298954

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